

Resonant leaky modes in all-dielectric metasystems: Fundamentals and Applications

Lujun Huang^{1,2}, Lei Xu³, David Powell¹, Willie Padilla⁴, Andrey E Miroshnichenko^{1*}

1. School of Engineering and Information Technologies, University of New South Wales, Canberra, ACT, 2600, Australia
2. School of Physics and Electronic Science, East China Normal University, Shanghai, 200241, China
3. Advanced Optics and Photonics Laboratory, Department of Engineering, School of Science and Technology, Nottingham Trent University, Nottingham NG11 8NS, United Kingdom
4. Department of Electrical and Computer Engineering, Duke University, Durham, North Carolina 27705, USA

Corresponding author: andrey.miroshnichenko@unsw.edu.au

All-dielectric metamaterials and metasurfaces have been demonstrated as ideal platforms to manipulate electromagnetic waves and enhance light-matter interaction. Analogous to guided modes in a dielectric waveguide, high refractive index dielectric metasurface supports leaky modes (also known as quasi-normal modes), including electric and magnetic resonant modes, which are represented by a complex eigenfrequency. Such leaky modes play a dominant role in governing the optical properties of dielectric nanoparticles and metasurfaces (i.e., absorption, scattering and emission). These unique properties enable researchers to design dielectric metasurfaces with desired functionalities without resorting to computationally expensive parameter scanning with full-wave simulation. Moreover, leaky modes underpin many exciting topics, such as Fano resonances, bound states in the continuum (leaky modes with $Q=+\infty$), coherent perfect absorption, parity-time symmetry, and exceptional points. This review provides an overview of the recent progress on leaky modes of all-dielectric-based metasystem, from fundamental physics to their applications. We start with surveying the fundamental physics of leaky modes and discussing leaky mode engineering in either a passive or active way. Then, we discuss the recent progress on the leaky modes' application in the perfect light absorber, solar cells, photodetectors, enhanced light emission and lasing, strong coupling, enhanced nonlinear harmonic generation, and structural color. Next, we present an overview of recent advances in bound states in the continuum and their application in enhanced light-matter interactions. Also, we review other interesting topics: parity-time symmetry and exceptional points, and discuss their application in manipulating light in an unprecedented way. Finally, we present our vision of the challenges and opportunities in this rapidly developing field of research.

1. Introduction

In 1908, Gustav Mie derived the analytical solution of a single dielectric particle made of high-index semiconductors with regular shapes like two-dimensional (2D) cylinders and three-dimensional (3D) spheres by solving Maxwell equations^{1–3}. He found a series of resonant peaks in the absorption and scattering cross-section spectrum, which are termed as Mie resonance to recognize his outstanding contributions to optics and photonics. Thanks to the significant advancement of modern nanofabrication technology, Mie resonance has been reinvigorated in the past two decades and found great success in controlling and manipulating light in an unprecedented way. Similar to metallic nanostructures supporting plasmonic resonances, high-index dielectric nanostructures support multipolar electric and magnetic Mie resonances, providing much freedom to control the light-matter interaction at a subwavelength scale. Besides, they have much lower losses compared to noble metals like silver and gold. These two extraordinary properties enable researchers to develop high-performance nanophotonic devices, such as metalens, low-threshold nanolasers, light-emitting diodes, solar cells, and photodetectors. The rich library of dielectrics, including Si, Ge, GaAs, AlGaAs, GaN, TiO₂, and Si₃N₄, allows researchers and scientists to design these photonic devices operating from ultraviolet, visible, near-infrared, mid-infrared to terahertz wavelength range. Moreover, all-dielectric metasystems, particularly all-silicon metasurface, are compatible with CMOS fabrication processes, making it possible to develop integrated photonic circuits. In the past decade, there have been many excellent reviews on all-dielectric metamaterials and metasurface^{4,5,14–16,6–13}, which cover either wavefront manipulation or Mie-resonance enhanced light-matter interactions.

Essentially, each Mie resonance in the dielectric structures can be perfectly linked with an eigenmode, also named a leaky mode or quasi-normal mode (QNM)^{17,18}. It has been demonstrated that the leaky modes provided by a single or an array of dielectric nanoparticles (NPs) govern the optical properties (i.e., scattering/absorption) of structures. Note that dielectric structures are not the only platform to support leaky modes or QNMs. Generally speaking, leaky modes exist in any open non-Hermitian systems, including but not limited to plasmonic NPs and metasurfaces, dielectric NPs and metasurfaces, coupled ring or disk resonators and waveguides as long as they interact with exterior environment. It has been well established in the text book of quantum mechanics that Hermitian Hamiltonians give rise to the real eigenvalues or eigen-energies and orthogonal eigen-basis. However, the boundary condition in many photonic and acoustic systems like metasurfaces are open at least in one dimension. Consequently, their Hamiltonians are non-Hermitian, leading to the complex eigenvalues of eigenmodes that are the typical features of leaky modes. As a particular type of leaky modes with an infinite quality-factor (Q-factor), bound states in the continuum (BICs) have attracted considerable attentions in both fundamental physics and practical applications. Besides, many other interesting physics and applications related to non-Hermitian photonics, such as parity-time (PT) symmetry and exceptional points (EPs), have been explored and demonstrated by tailoring the loss and gain of the system. The fundamental physics behind them can be attributed to the leaky modes engineering. Given the importance and powerful capabilities of the leaky modes, we review the all-dielectric metasystem from the leaky modes' perspective. In section 2, we first discuss the fundamental physics behind leaky modes, including the definition and calculation of leaky modes, and then reveal the vital role of leaky modes played in dictating the optical properties of all-dielectric metastructures from temporal

coupled-mode theory (CMT). After verifying the key role of leaky modes, we discuss several methods of engineering leaky modes. Then, we present an overview of leaky mode applications in perfect light absorption, solar cells, photodetectors, enhanced light emission and lasing, strong coupling, enhanced nonlinear harmonic generation, and structural color. In section 3, we review the most recent progress of BICs which are special leaky modes with an infinite Q-factor, including the fundamental physics behind BICs and their applications in enhanced light-matter interactions. In section 4, as the byproduct of leaky mode coupling, we survey the recent advances of PT-symmetry and EPs and their applications in lasers, laser-coherent perfect absorbers, and sensors. Section 5 concludes and presents an outlook of challenges and potential opportunities in all-dielectric nanophotonics.

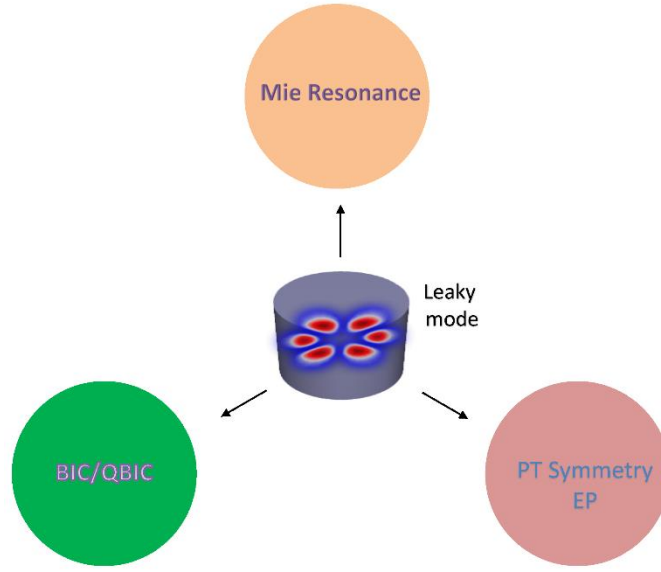


Fig.1. Resonant leaky modes can be linked to many interesting topics, including Mie resonances, BICs/QBICs, PT-symmetry and EPs in an open all-dielectric metasystem.

2. Leaky modes in all-dielectric structures and their applications

A non-hermitian system supports a series of leaky modes or QNMs because it strongly interacts with the exterior environment due to the open boundary. Typical examples include a single or an array of metallic or dielectric structures, or hybrid dielectric-metallic systems. This work mainly focuses on the all-dielectric structure, as shown in Fig.2.

Before we start discussing leaky modes, it is necessary to revisit the concept of guided modes, which share some similar features with leaky modes but have totally different physics and applications. We use a multilayer slab structure as an example to illustrate the difference between guided modes and leaky modes (See Fig.3a-b). Guided modes are sustained only when the refractive index of the core layer is larger than the top and bottom layer ($n_2 > n_1$ in Fig.3). Assuming the top and bottom layers have the same refractive indices, then eigenfunction in the core layer is a propagating wave while it shows exponential decay in the upper and down regions. The dispersion relationship can be obtained analytically by solving the Maxwell equation, which has been

explicitly discussed in many text books, see Yariv et al¹⁹. Fig.3e shows a typical eigenfield distribution inside and outside the waveguide region. It is clearly seen that outside the high-index core layer the eigenfield decays exponentially to zero in the far-field while it satisfies sine or cosine function inside the core layer depending on the parity of the guided modes. The formation of guided modes in such a structure can be explained intuitively from geometry optics perspective. The eigenfield inside the core layer can be represented by a superposition of two plane waves. One can be regarded as the incident wave while the other is the reflected wave. The incident wave experiences total internal reflection at the interface due to $n_2 > n_1$, ensuring the field confinement inside the core layer. However, only satisfying the total internal reflection does not guarantee the formation of guided modes. The accumulated phase in a round trip must be an integral multiple of 2π . This unique perspective reminds us that guided modes shall be excited by the endfire coupling at the end of the waveguide. One may use a similar way to explain the formation of guided modes in the cylindrical waveguide, as schematically shown in Fig.3c. The only difference is that the eigenfields inside and outside the core layer are Bessel functions. More detailed discussions can be found in the text books¹⁹, and we shall not repeat them here.

Unlike the guided modes, the eigenfields of leaky modes outside the high-index core layer propagates to infinity instead of decaying exponentially in the far-field (see Fig.3f). For the multilayer slab structure in Fig.3b, the eigenfrequencies and eigenfields of leaky modes can be solved analytically, as discussed in the following section. A leaky mode is characterized by a complex eigenfrequency $\omega = \omega_0 - i\gamma$, where ω_0 and γ are the resonant frequency and radiative decay rate of leaky modes, respectively. Its eigenfield should satisfy the out-going boundary condition so that the energy leaks out from resonators. It also shows divergence at $|r| \rightarrow \infty$ due to its complex eigenfrequencies, as confirmed in Fig.3f. Since the eigenfields are propagating wave in the far-field, according to the reciprocal theorem these leaky modes can be excited by an external source (i.e., plane wave or structured beam). Under such circumstances, the total internal reflection is no longer satisfied. A similar analysis also works for leaky modes in a single circular wire, as schematically shown in Fig.3d. Thus, we can conclude that the same structure can support both guided modes and leaky modes. However, the excitation method is different for guided modes and leaky modes due to the different formation mechanisms. As a result, they cannot be excited simultaneously, and only one can be excited by the corresponding excitation way. Another way to distinguish guided modes and leaky modes is to check whether the dispersion relationship is below or above the light cone because the guided (leaky) mode is below (above) the light cone. This section reviews the fundamental physics of leaky modes in all-dielectric metastructures and their applications in enhancing light-matter interaction.

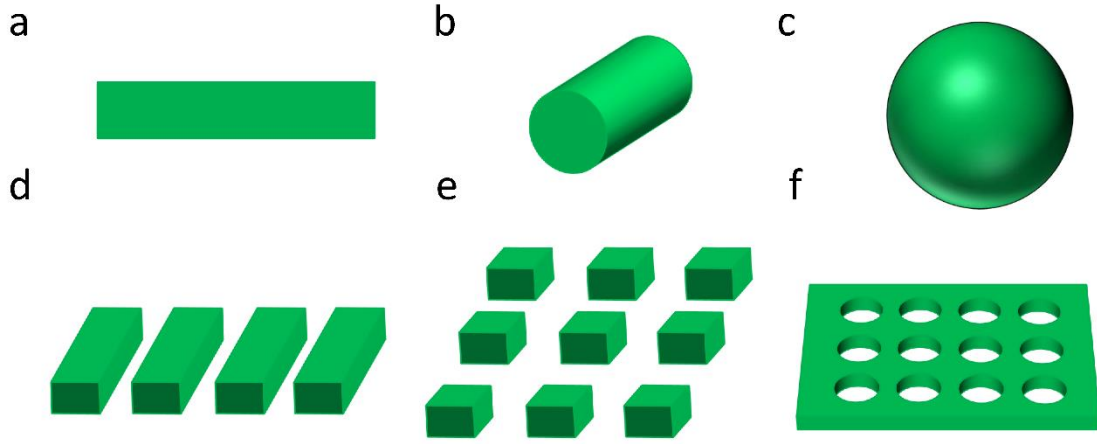


Fig.2. Schematic drawing of all-dielectric-based open systems. (a) 1D dielectric slab; (b) 2D dielectric cylinder; (c) 3D dielectric sphere; (d) all-dielectric metagrating; (e) all-dielectric metasurface made of an array of cuboid structures; (f) photonic crystal slab.

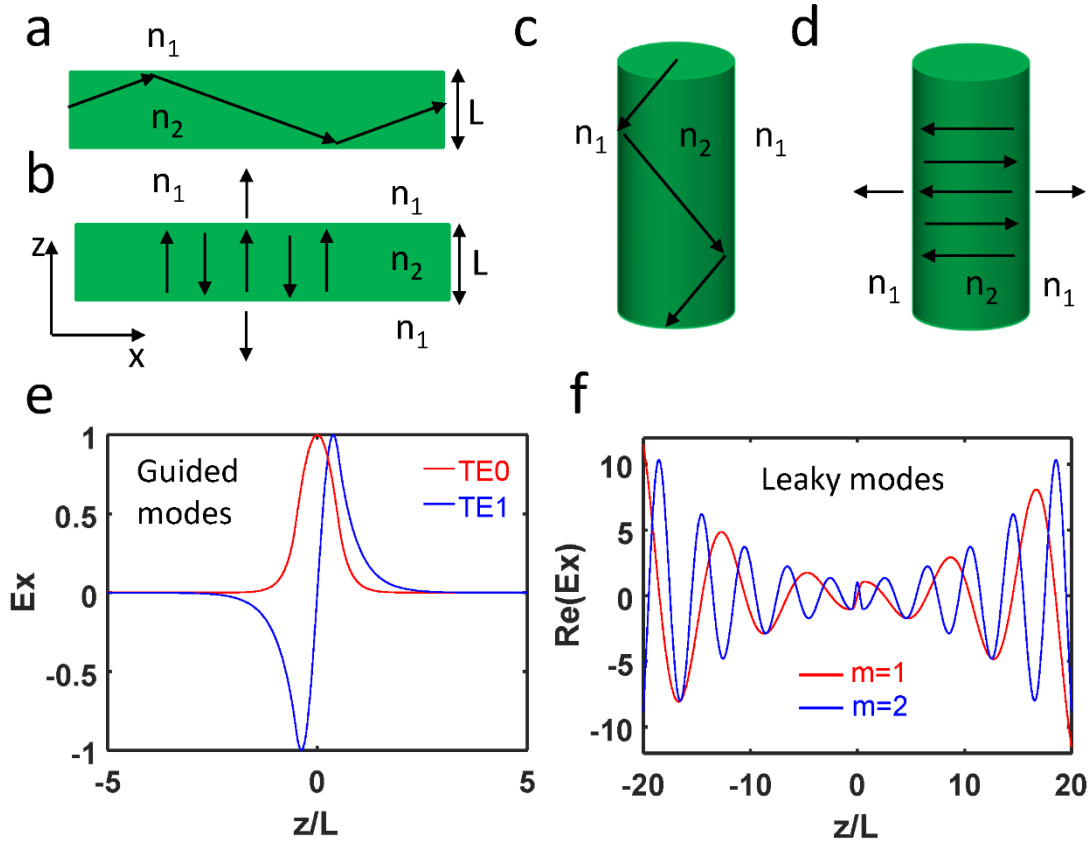


Fig.3. Comparison between guided modes and leaky modes. (a-b) Schematic drawing of guided modes (a) and leaky modes (b) in a 1D slab; (c-d) Schematic drawing of guided modes (c) and leaky modes (d) in a 2D dielectric cylinder; (e) Eigenfield distribution of the first two guided modes in a 1D slab with $n_1=1$ and $n_2=4$. The thickness of the slab is 300nm and the operating wavelength is $1.55\mu\text{m}$; (f) Eigenfield distribution of the first and second leaky modes in 1D slab with $n_1=1$ and $n_2=4$.

2.1. Definition of leaky modes and coupled-mode theory

2.1.1 Leaky modes in dielectric structures

We start by investigating the leaky modes of three dielectric structures with regular shapes, including 1D slab (Fig.4a), 2D circular wire (Fig.4d) and 3D sphere (Fig.4h) because both complex eigenfrequency and eigenfield of their leaky modes can be solved analytically with Mie-theory by boundary matching condition or scattering pole approach²⁰⁻²² (See Appendix-A for detailed derivation). Assuming the dielectric structure with refractive index n_2 is embedded into a homogeneous background medium n_1 , their complex eigenfrequencies could be obtained by solving the following transcendental equations

$$1D \text{ even: } \frac{n_2+n_1}{n_2-n_1} = e^{in_2 kL} \quad (1a)$$

$$1D \text{ odd: } \frac{n_2+n_1}{n_2-n_1} = -e^{in_2 kL} \quad (1b)$$

$$2D \text{ TE } (H_z = 0): n_2 \frac{J'_m(n_2 k r_0)}{J_m(n_2 k r_0)} = n_1 \frac{H'_m(n_1 k r_0)}{H_m(n_1 k r_0)} \quad (2a)$$

$$2D \text{ TM } (E_z = 0): \frac{J'_m(n_2 k r_0)}{n_2 J_m(n_2 k r_0)} = \frac{H'_m(n_1 k r_0)}{n_1 H_m(n_1 k r_0)} \quad (2b)$$

$$3D \text{ TE } (E_r = 0): \frac{[n_2 k r \cdot j_m(n_2 k r)]'_{r=r_0}}{j_m(n_2 k r_0)} = \frac{[n_1 k r \cdot h_m(n_1 k r)]'_{r=r_0}}{h_m(n_1 k r_0)} \quad (3a)$$

$$3D \text{ TM } (H_r = 0): \frac{[n_2 k r \cdot j_m(n_2 k r)]'_{r=r_0}}{n_2^2 j_m(n_2 k r_0)} = \frac{[n_1 k r \cdot h_m(n_1 k r)]'_{r=r_0}}{n_1^2 h_m(n_1 k r_0)} \quad (3b)$$

Where k is the complex eigen-wavenumber of the leaky modes, L is the thickness of the slab, r_0 in Eqs.(2)-(3) are the radius of a 2D circular cylinder and 3D sphere, $J_m(x)$ and $H_m(x)$ are respectively the m -th order of Bessel function of the first kind and Hankel function of the first kind, and $j_m(x)$ and $h_m(x)$ are m -th order of spherical Bessel function of the first kind and spherical Hankel function of the first kind, respectively.

Except for the complex eigenfrequencies, their eigenfields can be calculated accordingly. One may find detailed derivations in Appendix. Note that the complex eigenfrequency calculated from Eqs. (1)-(3) is represented by $\omega = \omega_0 - i\gamma$, where ω_0 and γ are the resonant frequency and radiative decay rate of leaky modes, respectively. To make the applications of leaky modes as general as possible, we define the normalized complex eigenvalue $N = N_{real} + 1i \cdot N_{imag} = n_2 k a = n_2 \omega a / c$, where n_2 is the refractive index of dielectric structure, a is the feature size of the geometry (i.e., $a=L$ for slab and $a=r_0$ for 2D circular wire and 3D sphere) and c is the speed of light in the free space. Due to their unique shapes, the leaky modes have different definitions. For 1D slab, leaky modes are named as TEM_m , where m is the number of antinodes. For both 2D circular wire and 3D sphere, leaky modes are noted as TE_{ml} (or TM_{ml}), where m is the azimuthal mode number and l is the radial order number. Without loss of generality, we set the refractive index of the background medium and dielectric structure as $n_1=1$ and $n_2=4$, respectively. Figs. 4b, 4e, 4i show some leaky modes' complex eigenvalues in a 1D slab, 2D circular wire and 3D sphere. Additionally, we also plot the eigenfield-distributions of several leaky modes as examples to illustrate the definition of eigenmodes, as shown in Figs. 4c, 4f-g and 4i-j. The complex eigenvalues of leaky modes show an interesting dependence on the refractive index. From Fig.5, it could be easily found that the imaginary parts of leaky modes are quite sensitive to the refractive index of dielectric resonators.

Nevertheless, their real parts are almost unchanged with the varied index. The stable real parts can be intuitively understood by the resonant condition $n_2 kL = m\pi$. The large variation on the imaginary parts can be attributed to the reduced index contrast between dielectrics and background medium, which is air here.

For a single or several dielectric particles with irregular shapes, their eigenmode information could be obtained with either numerical methods like the resonant-state expansion method or commercial software COMSOL MULTIPHYSICS. In the case of an array of dielectric structures, their leaky modes are usually calculated by numerical methods or commercial software. However, there are still some theoretical works showing that the leaky modes could be solved in a semi-analytical way^{23–26}, including the resonant-state expansion method²⁶. In the next part, we discuss the numerical methods that have been developed for calculating the leaky modes in all-dielectric resonators.

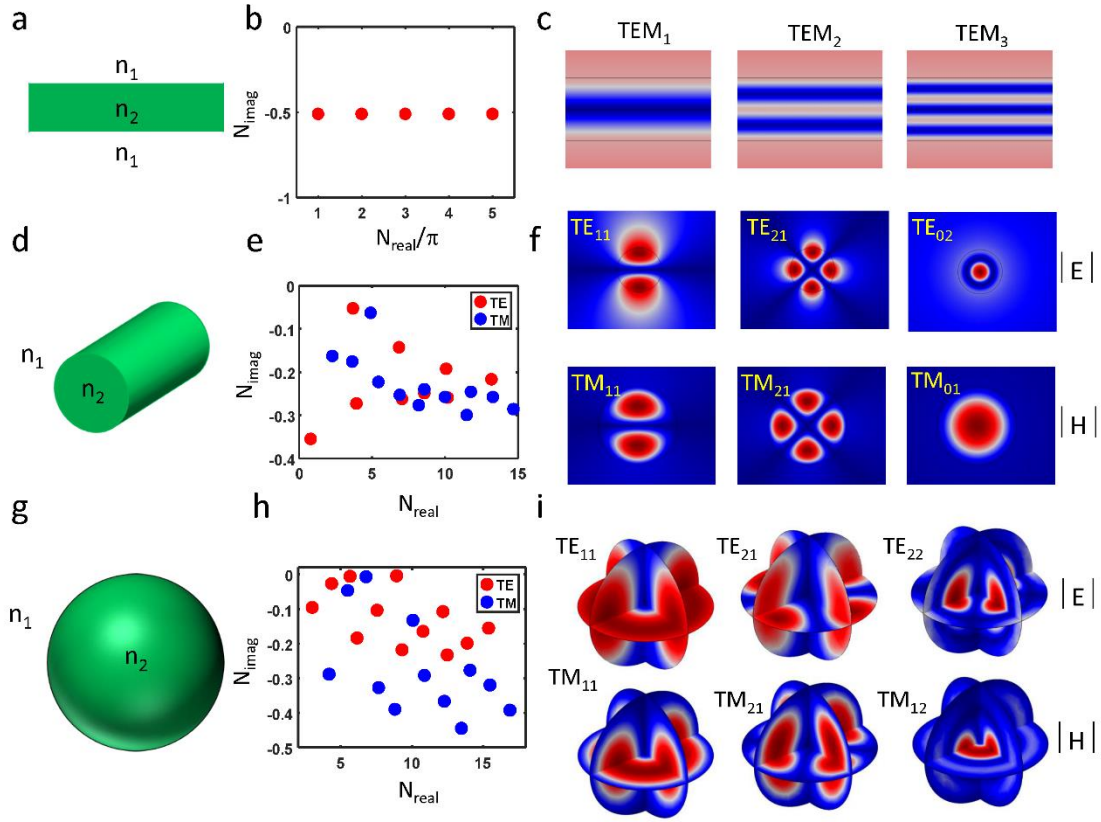


Fig.4. Leaky modes in a 1D dielectric slab, 2D dielectric cylinder and 3D dielectric sphere. (a) Schematic drawing of a 1D dielectric slab; (b) Complex eigenvalue of leaky modes in a 1D dielectric slab; (c) Eigenfield profile of modes TEM_1 , TEM_2 , TEM_3 . (d) schematic drawing of a 2D dielectric cylinder; (e) Complex eigenvalue of TE and TM leaky modes in a 2D dielectric cylinder; (f) Eigenfield profile of modes TE_{11} , TE_{21} , TE_{02} , TM_{11} , TM_{21} , TM_{01} . (g) schematic drawing of a 3D dielectric sphere; (h) Complex eigenvalue of TE and TM leaky modes in a 3D dielectric sphere; (i) Eigenfield profile of modes TE_{11} , TE_{21} , TE_{22} , TM_{11} , TM_{21} , TM_{12} .

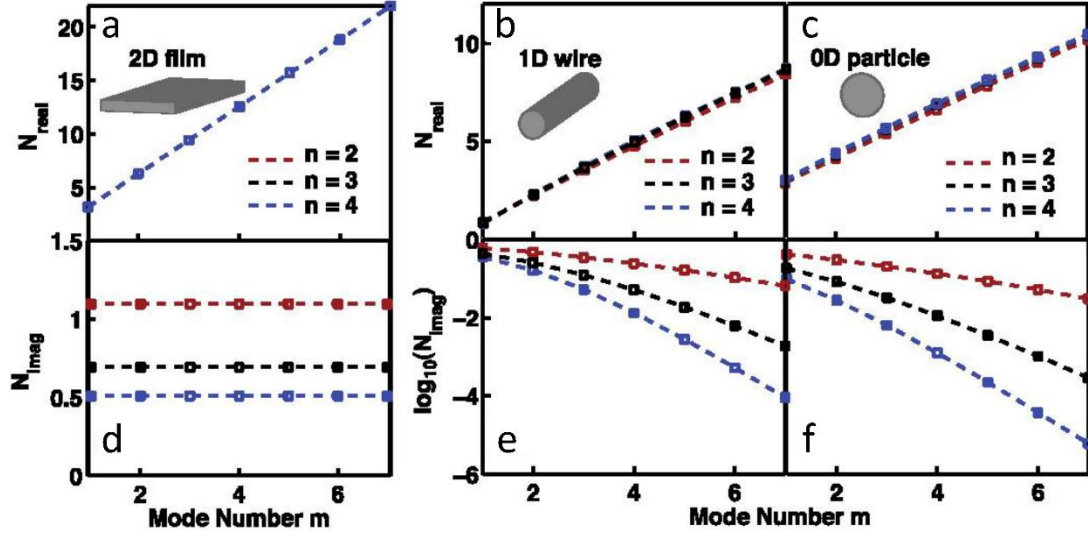


Fig.5. Leaky mode properties of a single dielectric structure, (a-c) Real part of eigenvalues for leaky modes supported by a 1D dielectric slab (a), a 2D dielectric cylinder (b) and a 3D dielectric sphere (c); (d-f) Imaginary part of eigenvalues for leaky modes supported by a 1D dielectric slab (d), 2D dielectric cylinder (e) and 3D dielectric sphere (f). (a)-(f) from Ref ²⁰.

2.1.2 Temporal Coupled Mode Theory

The powerful capability of leaky modes is that they play a dominant role in governing the optical properties (i.e., scattering, reflection/transmission and absorption) of dielectric structures^{20,21,27–30}, which is manifested by the temporal coupled-mode theory (CMT). Generally speaking, temporal CMT treats the structure as an optical resonator, and describes the optical response of the structure in terms of coupling between the incident wave and resonant modes supported by the structure. In the past three decades, temporal CMT has been successfully applied in describing the scattering (reflection, transmission) and absorption in both plasmonic and dielectric nanostructures. Here, we first review the application of temporal CMT in modelling the optical properties from a single or an array of NPs.

Case 1: Temporal CMT in a single NP

When a plane incident wave impinges on a 2D scatterer, part of the light is absorbed, and part of the light is scattered²⁷. According to Mie's theory, the scattering wave can be expressed as a function of the first kind of Hankel function. Considering the TM ($H//z$) incidence as an example, the total magnetic field outside the structure could be expressed as^{2,31}

$$H_{total} = \sum_{m=-\infty}^{\infty} H_0 [s_m^- H_m^1(kr) + s_m^+ H_m^2(kr)] e^{im\theta} \quad (4)$$

where H_0 is a normalized constant, $H_m^1(kr)$ and $H_m^2(kr)$ are m -th Hankel functions of the first and second kinds, and represent the outgoing and incoming waves, respectively. If the size of the scatterer falls within the subwavelength scale or the scatterer has cylindrical symmetry, the m -th outgoing wave is excited by the same order incoming wave. Thus, the reflection from m th channels is defined as

$$R_m = \frac{s_m^-}{s_m^+}. \text{ Applying energy conservation indicates } |R_m| \leq 1.$$

Because the dielectric cylinder is excited by plane wave incidence, the total magnetic field also could be expressed as follows

$$H_{total} = H_0 (e^{ik \cdot r} + \sum_{m=-\infty}^{\infty} i^m S_m H_m^1(kr) e^{im\theta}) \quad (5)$$

Where S_m is the scattering coefficient.

By expanding the plane wave as a superposition of Hankel functions and combining Eqs. (4) and (5), we have

$$R_m = 2S_m + 1 \quad (6)$$

After calculating the absorbed and scattered power from m -th channels, their corresponding absorbing, scattering and extinction cross-sections could be calculated as

$$C_{sm} = \frac{2\lambda}{\pi} |S_m|^2 \quad (7a)$$

$$C_{am} = -\frac{2\lambda}{\pi} (\text{Re}\{S_m\} + |S_m|^2) \quad (7b)$$

$$C_{em} = C_{sm} + C_{am} = -\frac{2\lambda}{\pi} \text{Re}\{S_m\} \quad (7c)$$

Eq.(7a) indicates that the maximum scattering cross-section by a single channel is $\frac{2\lambda}{\pi}$. However, there is no limit to the total scattering cross-section. The total scattering cross-section at a given wavelength can be boosted by arranging multiple channels into a single resonance through a core-shell structure that is made of metal-dielectric-metal, as demonstrated by Ruan et al.³².

Temporal CMT established the relationship between the reflection and leaky modes²⁷. It considered the scattering behaviour from an obstacle as the result of coupling between incidence and resonant modes supported by the structure. Part of the incoming waves is coupled into the resonator while the rest is directly reflected back into the background. The outgoing wave is contributed by the direct reflectance of incidence and coupling from the resonator. Its dynamics could be expressed as follows

$$\frac{dc}{dt} = (-i\omega_0 - \gamma_0 - \gamma)c + \kappa s^+ \quad (8a)$$

$$s^- = Bs^+ + \eta c \quad (8b)$$

Where c is the resonance's amplitude, ω_0 is the resonant frequency of leaky mode, γ_0 and γ are the intrinsic loss rate and radiation decay rate of leaky mode, respectively. $\kappa(\eta)$ represent the coupling between incoming (outgoing) wave and resonator. B is the background reflection constant. Rigorously speaking, temporal CMT is valid only when $\gamma_0 + \gamma \ll \omega_0$. For lossless structure, $B = e^{i\varphi}$

By applying energy conservation and time reverse symmetry, one can have $\kappa = \eta, \eta\eta^* = 2\gamma$.

Substituting them into Eq. (8) gives

$$R_m = \frac{s_m^-}{s_m^+} = \frac{i(\omega_0 - \omega) + \gamma_0 - \gamma}{i(\omega_0 - \omega) + \gamma_0 + \gamma} e^{i\varphi} \quad (9)$$

Then, combining Eq. (6) and Eq. (9) gives

$$S_m = \frac{1}{2} \left[\frac{i(\omega_0 - \omega) + \gamma_0 - \gamma}{i(\omega_0 - \omega) + \gamma_0 + \gamma} e^{i\varphi} - 1 \right] \quad (10)$$

By substituting Eq. (10) into (7), we could immediately have scattering and absorption cross-section as follows

$$C_{sct} = \frac{\lambda}{2\pi} \left| \frac{[i(\omega_0 - \omega) + \gamma_0](e^{i\varphi} - 1) - \gamma(1 + e^{i\varphi})}{i(\omega_0 - \omega) + \gamma_0 + \gamma} \right|^2 \quad (11a)$$

$$C_{abs} = \frac{2\lambda}{\pi} \frac{\gamma_0 \gamma}{(\omega_0 - \omega)^2 + (\gamma_0 + \gamma)^2} \quad (11b)$$

Eq.(11) shows that the absorption cross-section spectrum has a Lorentz profile and does not depend on the background scattering phase φ . On the contrary, the line shape of the scattering cross-section is quite sensitive to the φ . It has a Fano profile with asymmetric line-shapes³³ unless $\varphi=0$ or π . This also

suggests an effective way of engineering the line shape of the scattering spectrum from a single NP. Furthermore, the absorption cross-section contributed by a single mode reaches maximum $\frac{\lambda}{2\pi}$ only when the on-resonance critical coupling is satisfied $\gamma_0 = \gamma$.

Following a similar process, one could derive the expressions of absorption and scattering cross-section in a single 3D NPs³⁴. The only difference is that the spherical Hankel function should be used. As such, we do not repeat them here and directly give the final expression for a single 3D NP as follows

$$C_{sl} = (2l + 1) \frac{\lambda^2}{2\pi} \left| \frac{R_{l,p}-1}{2} \right|^2 \quad (12a)$$

$$C_{al} = (2l + 1) \frac{\lambda^2}{8\pi} (1 - |R_{l,p}|^2) \quad (12b)$$

$$R_{l,p} = \frac{i(\omega_0 - \omega) + \gamma_0 - \gamma}{i(\omega_0 - \omega) + \gamma_0 + \gamma} e^{i\varphi} \quad (12c)$$

Where l is the order of spherical Hankel function, p represents the polarization and could be TE or TM.

Similar to the 2D case, there is an upper limit $(2l + 1) \frac{\lambda^2}{2\pi}$ for scattering cross-section in a single channel. Here, it is worth noting again that the contribution of a single channel to scattering cross-section has an upper limit. However, there is no constraint on the total cross-section. In principle, one can achieve an arbitrarily large scattering cross-section by bringing multi-channels' contribution closer to one resonance. This superscattering phenomenon was theoretically confirmed in a subwavelength nanosphere made of plasmonic-dielectric-plasmonic materials by Ruan et al³⁴, where resonance is generated in a large number of channels. It was experimentally demonstrated recently by Qian et al.³⁵.

Case 2: Temporal CMT in 2D metasurface and photonic crystal slab

Temporal CMT has a slightly different form in describing the light-matter interaction of metasurface and photonic crystal slab because there are two ports in both input and output channels^{29,36}, as shown in Fig.6a. Considering a lossless slab that supports a single mode as an example, the coupling between the resonator and external excitation could be described as

$$\frac{dc}{dt} = (-i\omega_0 - \gamma)c + (\kappa_1 \quad \kappa_2) \begin{pmatrix} s_1^+ \\ s_2^+ \end{pmatrix} \quad (13a)$$

$$\begin{pmatrix} s_1^- \\ s_2^- \end{pmatrix} = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \begin{pmatrix} s_1^+ \\ s_2^+ \end{pmatrix} + \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} c \quad (13b)$$

Where c is the amplitude of resonance, ω_0 and γ correspond to the leaky mode's resonant frequency and decay rate, respectively. $s_{1,2}^+, s_{1,2}^-$ are the incoming (outgoing) wave from ports 1 or 2.

The scattering matrix S could be obtained by solving Eq. (13),

$$\begin{pmatrix} s_1^- \\ s_2^- \end{pmatrix} = S \begin{pmatrix} s_1^+ \\ s_2^+ \end{pmatrix} = \left[\begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} + \frac{\begin{pmatrix} d_1 \\ d_2 \end{pmatrix} (\kappa_1 \quad \kappa_2)}{i(\omega_0 - \omega) + \gamma} \right] \begin{pmatrix} s_1^+ \\ s_2^+ \end{pmatrix} \quad (14)$$

By checking the energy conservation and performing time-reversal symmetry, we will have

$$\kappa_1 = d_1, \kappa_2 = d_2 \quad (15a)$$

$$|d_1|^2 + |d_2|^2 = 2\gamma \quad (15b)$$

$$\begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \begin{pmatrix} d_1^* \\ d_2^* \end{pmatrix} = - \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} \quad (15c)$$

The self-consistency of temporal CMT is verified by proof of the unitary property of the scattering matrix.

Considering the structure having vertical mirror-symmetry, $d_1 = \pm d_2$, $+$ ($-$) represents even (odd) mode. By choosing the appropriate reference plane, the scattering matrix B from direct background reflection could be further simplified as

$$B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} = \begin{pmatrix} r & jt \\ jt & r \end{pmatrix} \quad (16)$$

Where both r and t are real with $r^2 + t^2 = 1$

Combining Eqs. (14)-(16) gives us

$$S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = \begin{pmatrix} r & jt \\ jt & r \end{pmatrix} + \frac{\gamma}{i(\omega_0 - \omega) + \gamma} \begin{pmatrix} -(r \pm jt) & \mp(r \pm jt) \\ \mp(r \pm jt) & -(r \pm jt) \end{pmatrix} \quad (17)$$

From Eq. (17), one can find that $S_{11} = S_{22}$, $S_{12} = S_{21}$ due to mirror-symmetry and time reversibility. Then, reflection (or transmission) could be easily computed by $R = |S_{11}|^2$ and $T = |S_{21}|^2$. Fan et al demonstrated that the nonzero background reflection or transmission induces the Fano resonance with asymmetric lineshape in reflection or transmission spectrum²⁹. For a slab with intrinsic loss, it is not difficult to derive the absorption efficiency of a single mode based on temporal CMT, which has the following expression

$$A = \frac{2\gamma_0\gamma}{(\omega_0 - \omega)^2 + (\gamma_0 + \gamma)^2} \quad (18)$$

From the above equation, it can be easily observed that absorption of a single resonance reaches its maximum 50% when intrinsic absorption rate is balanced by the radiation decay rate at resonant frequency³⁷, corresponding to the critical coupling conditions. If the single resonance is supported by a layer of infinitesimal thickness, then the resonance must be of even symmetry³⁷. Otherwise, a relatively thick layer ($t \sim \lambda/2$) may support both even (electric) and odd (magnetic) single resonances. The absorption could be enhanced to unity by placing a conductor closely behind the lossy slab at a specific distance to create an additional resonance of odd symmetry. In this scenario the even mode and odd mode each contribute 50% absorption, bringing about 100% total absorption. Another approach is to use a single structure, e.g. an all-dielectric metasurface, which supports two degenerate modes of opposite symmetry with identical resonant frequencies and matched material and radiative decay rates³⁸. On the other hand, perfect coherent absorption may be realized through in-phase (even mode), or out-of-phase (odd mode), illumination from two sides, and simultaneous satisfaction of the critical coupling condition on resonance. Since a coherent absorber is either even or odd, it absorbs 100% of the incident coherent radiation or, equivalently, 50% of incoherent radiation³⁹. These three strategies of electromagnetic wave absorption will be discussed in a later sub-section. Note that Eqs. (16)-(18) only strictly apply to a photonic crystal slab or metasurface which is embedded in a symmetric environment. Asymmetric configurations, with respect to the middle-plane of the layer, are considered by Wang et al⁴⁰.

In summary, temporal CMT perfectly correlates the absorption and scattering cross-section in a single 2D and 3D structure, or reflection (transmission) and absorption with a complex eigenfrequency of resonant mode. The powerful capability of temporal CMT has been confirmed in many works. Fig.6 shows several examples of temporal CMT used for reproducing either the absorption or reflection in a single dielectric nanostructure and photonic crystal slab. Here, it is noteworthy that the total absorption could be calculated by summing up the absorption from all leaky modes because absorption only depends on the eigenmode information, but does not involve the phase arising from background

scattering. With the information of the complex eigenvalue of leaky modes in Fig. 4, Yu et al. successfully reconstructed the total absorption spectrum of a continuous slab, a single cylinder and a sphere²⁰ (Fig.6b), showing a nice agreement with the analytical solutions based on Mie theory. Reproducing the scattering matrix of a single, array of dielectric NPs and photonic crystal slab becomes complicated and challenging as it requires both complex eigenfrequency and scattering from the direct transport process. Alpegiani et al. revealed that reflection and transmission could be retrieved by taking account of complex eigenfrequencies and far-field information of all relevant leaky modes³⁰ (Fig.6c-d). The scattering cross-section from a single dielectric cylinder and sphere is tackled with temporal CMT by Yu et al.²¹, where the background reflection phase is derived analytically. The relevant result is presented in Fig.6e. For an NP with an irregular shape, Yan et al. found that both leaky modes (or QNMs) and perfectly matched layer modes have to be considered to reproduce the scattering and absorption cross-section⁴¹. Perfectly matched layer modes are particularly important for a metallic NP on the semiconductor substrate. Since this review focuses on the leaky modes in an all-dielectric structure, leaky modes in a plasmonic resonator or hybrid plasmonic-dielectric resonator are beyond the scope of this review. Readers may refer to two comprehensive reviews written by Lalanne et al.¹⁷ and Kristensen et al.¹⁸, respectively. Before ending the discussion of this section, we would like to reiterate that temporal CMT has demonstrated its powerful capability in predicting some interesting phenomena like antireflection coating layer⁴², superscattering^{32,34}, and complete polarization conversion^{43,44}. They also enable the design of high-performance photonic and optoelectronic devices, such as solar cells and photodetectors, which are discussed in the later section.

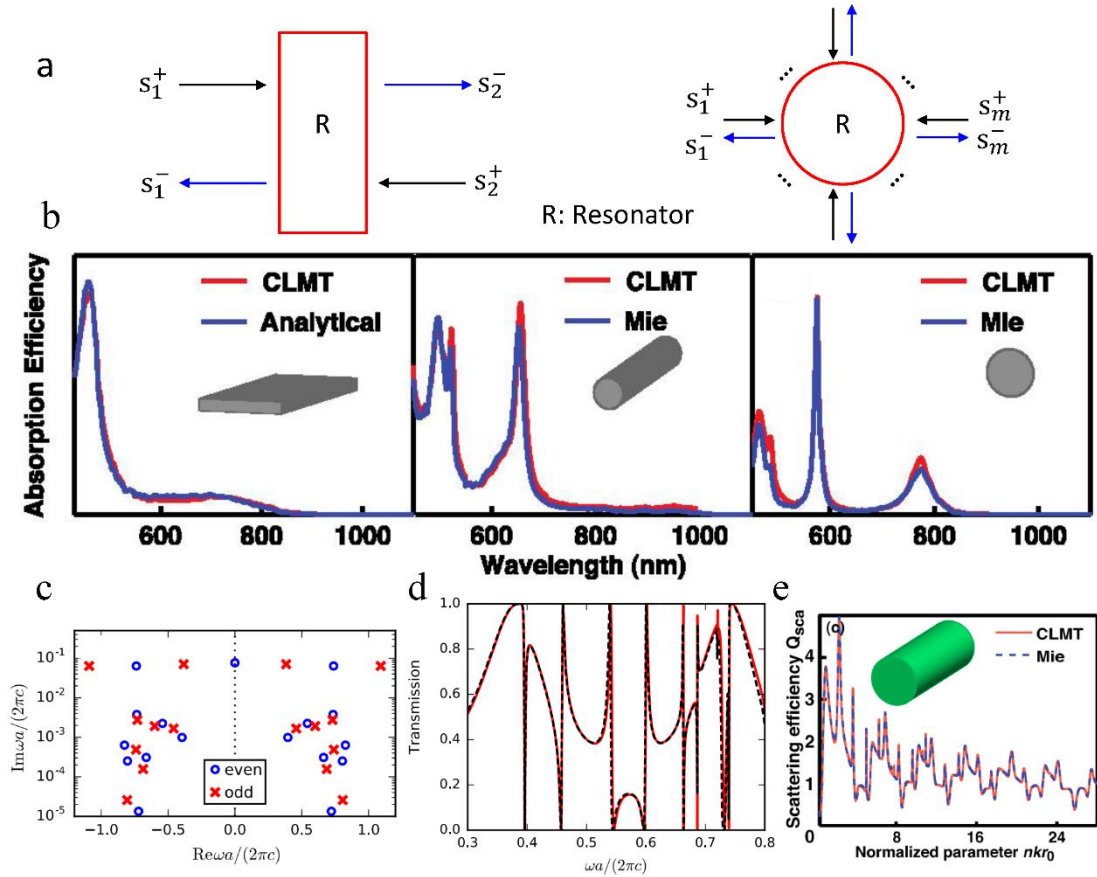


Fig.6. (a) Schematics of an optical resonator coupled with one port and two ports. (b) Absorption efficiency in a 1D dielectric slab, 2D dielectric cylinder, and 3D dielectric sphere calculated by temporal CMT and analytical

method. (c) Complex eigenvalues of leaky modes supported by a Si photonic crystal slab. (d) Transmission calculated by QNMs expansion and RCWA. (e) Scattering efficiency of a single dielectric wire calculated by temporal CMT and Mie theory. (b) from Ref ²⁰. (c)-(d) from Ref ³⁰. (e) from Ref ²¹.

2.2. Numerical methods for calculating leaky modes

For an open resonator with regular geometries such as spheres^{20,45}, cylinder²⁰, or Fabry-Perot resonators¹⁷, solutions for scattered fields are available in closed form (See Appendix-A), which can readily be adapted to find modes. However, in practice more complex geometries are of interest, so numerical methods must usually be applied. In open systems, with radiation boundary conditions, Maxwell's equations become non-Hermitian. The most important consequence of this is that the modal fields no longer satisfy the usual orthogonality relationships. The eigenfrequencies are complex, $\omega_n = \omega'_n - i\omega''_n$, with the imaginary part of passive objects occurring at $\omega''_n < 0$ when using the time convention $\exp(-i\omega t)$. Sommerfeld radiation conditions dictate that solutions in the far-field decay as $\exp(ikr)/4\pi r$, with $k = k' - ik'' = \omega/c$. Since $k'' < 0$, this leads to solutions which grow exponentially in the far-field. Although this result is initially counter-intuitive, it should be recalled that larger values of r , correspond to earlier values in time when the energy was radiated by the source. Since at the complex eigenfrequency the source strength diverges as $t \rightarrow -\infty$, the corresponding radiated fields must also diverge as $r \rightarrow \infty$. Further discussion of causality and convergence can be found in Ref ⁴⁶. This divergence means that the usual ortho-normality conditions do not apply, since they correspond to normalization of the energy in the field, which is unbounded. Instead, they satisfy a bi-orthogonality relationship with a set of adjoint modes, under an unconjugated inner product⁴⁷. This unconventional normalization is what gives rise to the term QNMs.

2.2.1 Semi-analytical approaches

A review of early work on QNMs can be found in Ref ⁴⁸. Initial techniques for studying open systems were based on the “system and bath” approach. Here, the problem is partitioned into two parts, the modes of which are solved separately, and then coupled together. The system (e.g. the internal part of the cavity, or the body of the dielectric resonator) is solved with closed boundaries, giving a discrete set of normal modes. The surrounding bath (e.g. free space) has a continuous spectrum of modes. This approach is in principle generally applicable, however in some cases the division between the system and the bath can be difficult, and the resulting formulation requires dealing with a continuous modal spectrum. QNMs are introduced as a more intuitive approach, allowing analysis to be performed with only a finite set of discrete modes of the entire system, enabling established techniques for closed systems to be applied to open resonators.

A contemporary, semi-analytical approach to finding QNMs is known as the resonant-state expansion²⁶. This approach starts with the eigen-solutions to a known scattering problem, such as a dielectric sphere, and applies perturbation theory to find the solution for other geometries. This approach has been used to demonstrate quasi-BICs (QBICs) for dielectric resonators⁴⁹ and their applications to nonlinear nanophotonics⁵⁰. The main drawback of this approach is the complexity of constructing the required perturbation matrices and the difficulty of incorporating background media other than free space, such as a substrate.

2.2.2 Boundary element approaches

Boundary element approaches are advantageous for open resonator problems since they solve only for the fields on the surface of the object (or equivalent surface currents). These fields remain finite at complex frequencies, thus they require no special treatment of diverging solutions. For metallic objects at microwave frequencies, which are treated as perfect electric conductors, this approach was originally referred to as the singularity expansion method and was primarily motivated by predicting time-domain features of a radar echo based on the resonant modes of a target⁵¹.

For dielectric objects, initial approaches have been suggested based on finding the minimum of the condition number or determinant of the system matrix⁵². More recently, integral approaches have been extended to plasmonic elements^{53,54} (Fig.7a-b), and all-dielectric meta-atoms⁵⁵(Fig.7c), where it was shown that the non-orthogonality of the resonator modes leads to interference between them. This can explain certain effects, such as the anapole moments, which lead to the suppression of dipolar radiation. Open-source solvers of QNMs based on the boundary element method can be found in Ref ^{56,57}.

In boundary element approaches, the system matrix always includes terms with high-order frequency dependence, thus regular eigenvalue solvers cannot be used to find the modes. Instead, iterative methods or contour integration must be used^{58,59}. This means that no special approach is required to deal with dispersive media, so long as their model can be continued analytically in the complex frequency domain (e.g. with a Drude-Lorentz model). For all numerical methods, it is important to distinguish between physically meaningful resonances of the structure, and purely numerical solutions introduced by the discrete operator. Appropriate choice of the integral operator can ensure that the unwanted numerical solutions are well separated from the true solutions in complex frequency space.

In many practical problems, the background medium of a nanoresonator is not free space. Instead, it may be located on a substrate (possibly with multiple layers), embedded within a waveguide, or placed within a more complex structure such as a photonic crystal. In such cases, it is necessary to use a more complex Green's function, which may not be available in closed form. Since some other numerical method, such as finite element, may be needed to find such Green's functions, in many cases it is simpler to use this method to directly solve for the QNMs.

2.2.3 Finite element approaches

Finite element methods (FEM) are often favoured in numerical solution of electromagnetic problems, due to their highly flexible mesh, and suitability to problems and geometries of almost arbitrary complexity. Since they require discretization of the entire computational domain, radiation conditions must be explicitly enforced at boundaries using techniques such as perfectly matched layers. The incorporation of such boundary conditions into an eigenvalue solver is one of the main complexities of using FEM to find QNMs. It has been shown that the normalization can be performed using only a volume integral over the entire computational domain, including the perfectly matched layer. This was used to calculate the Purcell factor for open optical resonators⁶⁰, where traditional methods typically fail due to the mode volume becoming unbounded.

One advantage of FEM approaches is that they lead to conventional eigenvalue problems in the case of non-dispersive media, since the system matrix does not depend on frequency. In many works, the use of dispersive media leads to a nonlinear eigenvalue problem. However, by incorporating auxiliary variables into the equation (corresponding to local polarization and its temporal derivatives), the system of equations becomes second order again. It has been shown that this leads to a conventional quadratic eigenvalue problem for the modes, and a form of the orthogonality relationship which is free

from frequency derivatives⁴¹. Fig.7d shows some typical QNMs of a silver bowtie antenna. Note that some controversy remains in the literature over the merits of different approaches to the normalization of QNMs^{17,61–63}. For the specific case of spherically symmetric geometries, recent work has shown that Gaussian regularization and the inclusion of non-resonant terms can together ensure convergence⁶⁴. An open-source Matlab script to find QNMs using the commercial finite element solver COMSOL Multiphysics can be found in Ref⁶⁵.

Summary

QNMs typically require custom solvers since they require unconventional approaches to their normalization and they do not obey the standard orthogonality relations. Semi-analytical approaches, boundary element method solvers and finite element solvers are the most commonly used, each with their own advantages and disadvantages. Other techniques have been applied, including the Fourier Modal Method⁶⁶, or from the singularities of the Scattering Matrix or T Matrix⁶⁷. In addition, in the literature, many eigenvalue-based techniques can be found, which solve a separate eigenvalue problem at each frequency. These approaches are not considered here, since the set of basis vectors that they yield vary with frequency, and thus do not constitute the physically meaningful resonances of the structure. For a more detailed summary of important considerations for QNMs solvers, the reader is referred to the review articles^{17,18}.

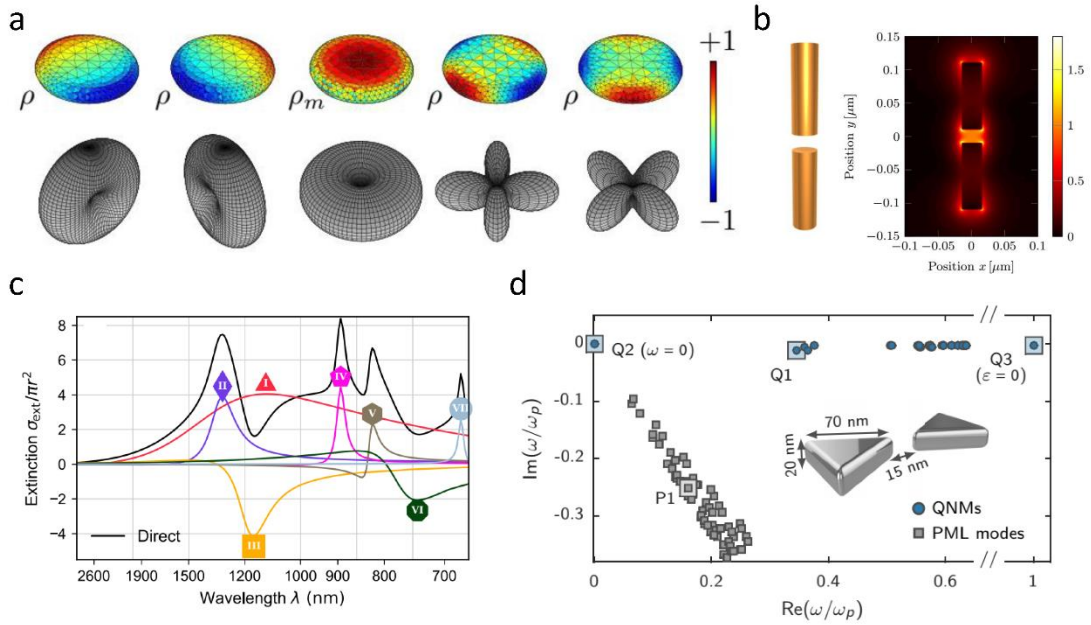


Fig.7. (a) QNMs of a plasmonic disc, showing charge distributions and far-field radiation patterns. (b) Electric field distribution of the fundamental QNMs of a gold nanorod dimer. (c) The extinction of a dielectric disk (black line) is decomposed into contributions from QNMs (colored lines). Note that some terms become negative, as the interference between modes can cancel radiation. (d) Complex eigenfrequencies of a bowtie nanoantenna (Q1, Q2, Q3). Note that the numerical scheme also introduces unphysical “perfectly matched layer modes”, which must be distinguished from physically meaningful QNMs. (a) from Ref⁵³. (b) from Ref⁶¹. (c) from Ref⁵⁵. (d) from Ref⁴¹.

2.3. Leaky Mode Engineering

As demonstrated in the previous section, leaky modes determine the optical properties of dielectric

nanostructures. Thus, the question of manipulating the light scattering and absorption is reduced to engineer the leaky modes supported by the different dielectric nanostructures. Currently, one can achieve the control of leaky modes in both passive and active ways^{68–71}. In this part, we discuss some recent efforts of engineering the leaky modes with various strategies.

2.3.1 Mode Engineering by Morphology

The typical way of engineering the leaky mode is to change the shape of the dielectric nanostructure. The previous section has described the leaky modes of the 1D circular nanowire (NW) and 3D spherical NP, whose solutions can be derived analytically from Mie theory. Benefiting from this, these two standard shapes provide an excellent playground to study fundamental physics. However, it is very challenging to tune the leaky mode property for such fixed shapes because the only parameter that can be tuned is the radius. Also, circular NW and spherical NP cannot be massively fabricated with standard nanofabrication technology. This might pose the challenge of developing commercial products based on them.

Dielectric nanostructures with rectangular cross-sections, such as rectangular NW, cuboid and nanodisk, may provide a good alternative as they can be fabricated on a large scale with electron beam lithography, laser interference lithography, and nanoimprinting technology. Also, these shapes provide more freedom to engineer the mode properties. Considering the case of single rectangular NW with a size ratio defined as $R=b/a$ (a is the width and b is the height of NW), it supports a series of transverse electric TE_{ml} modes ($E//z$) and transverse magnetic TM_{ml} modes ($H//z$), where m and l are the antinode number along the x and y directions. Huang et al. found that the real part of the eigenvalue ($N=n\omega b/c=N\omega_0 b/c=n\omega_0 b/c-i\gamma$), where ω_0 and γ are the resonant frequency and radiative decay rate of leaky modes, respectively, and c is the speed of light in free space) shows a linear dependence on the size ratio for relatively lower order modes TE_{ml}⁷² (Fig.8a-b), which can be expressed as $n\omega_0 b/c \approx (m-1)\pi + (l-1)\pi$. Such a linear relationship is well explained by the modified Fabry-Perot cavity model, in which the rectangular NW resonator is treated as the coupled Fabry-Perot cavities along x and y axes, whose coupling mainly arises from the nonideal truncated open boundary that may induce the phase discontinuity. It is noteworthy that this interesting phenomenon also happens in the case of TM_{ml} modes of rectangular NW and leaky modes of triangular NW, cuboid and disk. The simple relationship between the resonant frequency and size ratio provides unprecedented flexibility in controlling the optical properties of such dielectric structures. For example, both the absorption and scattering efficiency can be significantly enhanced by overlapping the resonant wavelength of two modes via merely tuning the size ratio. The first experimental⁷³ study on the rectangular NW and cuboid was done by Ee et al. in 2015. This work considered the cuboid nanostructure with a fixed width 60nm of square cross-section but changed lengths from 20nm to 1000nm. Such nanostructures support two leaky mode resonances TM₀₁ and TM₁₁ across the wavelength range from 400nm to 1000nm (Fig.8c-f). Here, it is necessary to point out that they adopt the definition of circular NW instead of the definition used above in rectangular NW. The resonant wavelength of mode TM₀₁ can be widely tuned over the entire visible wavelength range while the length of nanoblock changes from 150nm to 650nm. On the contrary, the leaky mode TM₁₁ has an almost unchanged resonant wavelength at 440nm. The completely different behaviors of the two modes are explained by the truncated waveguide dispersion controlled by the nanoblock length. Additionally, by overlapping two resonances, the scattering cross-section is significantly enhanced, and thus approaches the single-channel limits. The wide tunability of resonant scattering has also been used to develop the structural color measured by dark-field microscopy⁷⁴.

Besides the shape-induced leaky mode engineering, one can also achieve control over the leaky modes by introducing one or multilayer coating above the dielectric nanostructure. As we mentioned above, for a single circular NW or sphere NP, the only tuned parameter is their radius. The shell-coating brings two additional freedom (refractive index of coating material and shell thickness) to control the leaky modes in single dielectric nanostructures. Yu et al. demonstrated that the solar absorption could be significantly enhanced by the core-shell structure⁷⁵, consisting of an amorphous silicon core and lossless dielectric shell. Introducing the shell layer outside the absorption core structure not only enables the antireflection effect but also induces the multiplication of contribution from multiple leaky modes. Kim et al. demonstrated an improved light absorption by 40% in crystalline silicon core with 20nm amorphous silicon shell compared to homogeneous crystalline silicon NW⁷⁶. The large absorption enhancement results from the several leaky modes showing localized fields within the shell layer.

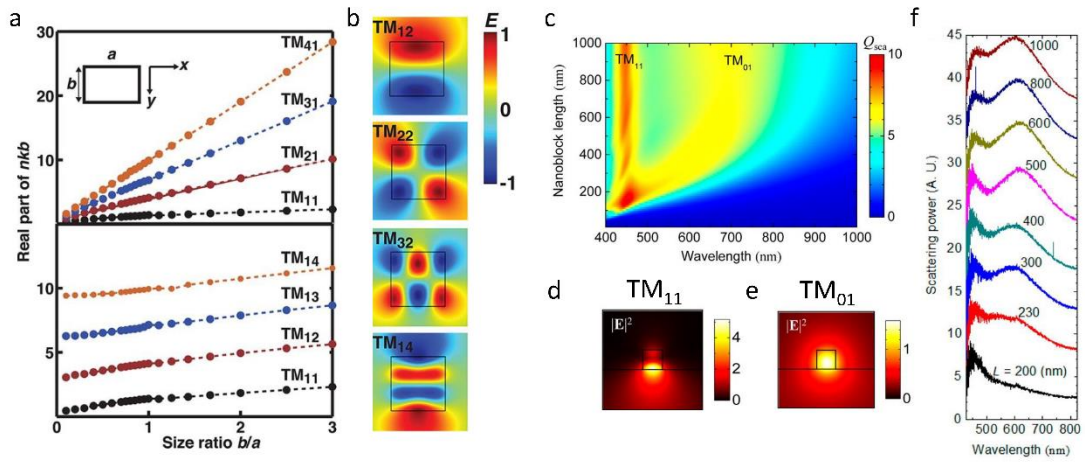


Fig.8. Leaky mode engineering by structure morphology. (a) Real part of eigenvalues of different leaky modes vs size ratio $R=b/a$; (b) Eigenfield distribution for leaky modes TM₁₂, TM₂₂, TM₃₂ and TM₁₄. (c) Scattering efficiency mapping as functions of incident wavelength and nanoblock lengths. (d)-(e) Scattered electric field intensity of Si NW ($a=b=60\text{nm}$) for leaky modes TM₁₁ ($\lambda_0=440\text{nm}$) (d) and TM₀₁ ($\lambda_0=725\text{nm}$) (e). (f) Measured scattering spectra of Si nanoblocks with varied lengths from 200nm to 1000nm. (a)-(b) from Ref ⁷². (c)-(f) from Ref ⁷³.

2.3.2 Mode Engineering by Substrate and Superstrate

Mie theory gives the exact analytical solution of dielectric NPs embedded into the homogeneous background medium. However, the dielectric NP should be placed on the substrate for most practical applications. The interaction between dielectric nanostructures and substrate could strongly modify resonant mode properties. Thus, the substrate may serve as another degree of freedom to tune the optical properties of dielectric nanostructures. Tremendous effort has been made to investigate the influence of the substrate on the leaky mode resonances.

Among the diverse substrates, the metallic substrate is one of the most frequently used substrates in nanophotonics. In the case of electrostatics, putting a positive charge above a flat metallic mirror is equivalent to creating a virtual negative charge. So, what happens if a single dielectric nanostructure is placed onto a metallic substrate like aluminum, gold and silver? Xifre-Perez et al. gave a definite answer to this question by studying the scattering spectrum from a single silicon nanosphere onto a gold substrate⁷⁷. Such a hybrid cavity-mirror system is equivalent to two coupled silicon spheres that only support leaky modes with anti-symmetric electric field distribution. Both the simulated and

experimental results show that the presence of mirrors remarkably modified the scattering spectrum of a single NP, resulting in amplified scattering at a certain wavelength. The enhanced scattering cross-section is linked to generating real and virtual electric dipole pairs, inducing an effective magnetic dipole resonance. One can also place the dielectric NP above a metallic mirror with an air-gap between them. In this regard, the air-gap can serve as a new degree of freedom to engineer the leaky modes. By placing the Si NW onto an aluminium-coated convex mirror, Holsteen et al. experimentally demonstrated the tunable electric and magnetic resonances by varying the height between NW and mirror⁷⁸. Also, they developed a nanoelectromechanical system to actively control the structural color by applying gating voltages.

Groep et al. conducted a comprehensive study on how the presence of substrate influences the electric and magnetic resonance supported by a single dielectric cylinder with finite thickness⁷⁹. Fig.9a shows the scattering cross-section of an isolated silicon cylinder on the substrate with a refractive index varying from 1 to 3.5. It is found that the increasing refractive index of substrates not only induces redshifts of resonant wavelength of both electric dipole (ED) and magnetic dipole (MD) resonances, but also broadens the resonant peaks, causing spectrum overlap between the ED and MD resonance. This can be intuitively understood by the additional leakage into the substrate because of the reduced refractive index contrast between nanostructure and substrate. Also, for a Si nanostructure with the same volume but different shapes (e.g, cylinder, sphere and cuboid), the simulated results indicate that the semi-infinite substrate with $n=3.5$ has larger effects on broadening both the resonant peak of ED and MD for cylinder and disk than the case of sphere due to the larger contacting area for the former two shapes comparing to the latter one. If a multilayer substrate is used, the ED and MD mode can be selectively enhanced by changing the thickness of spacing layer. Besides, the substrate brings an extra degree of freedom of realising the directional radiation for both ED and MD modes. Besides dielectric substrates, other substrates like hyperbolic metamaterials are also investigated by Markovich et al.⁸⁰. Another role of the substrate is to bring about magnetoelectric coupling and resonant bianisotropic interaction between electric and magnetic dipole mode (Fig.9b), as revealed by Miroshenichenko et al.⁸¹.

Supersubstrate, which is the material covering on top of the dielectric metastructure, plays a similar role in controlling the resonant modes' properties as substrates. The advantage of supersubstrate compared to a substrate is that it enables active tuning of the leaky modes of dielectric nanostructure by utilising the liquid crystal or novel epsilon near zero materials⁶⁸⁻⁷⁰. Liquid crystal (LC) experiences the transition from the nematic phase to the isotropic phase, accompanied by the refractive index change. Typically, there are two ways to induce such a transition: heating and electrical gating. The first experimental verification of active tuning of the leaky modes was done by Sautter et al. with all-dielectric silicon metasurfaces⁸². After fabricating a silicon nanodisks array, Licristal E7 LC from Merck is coated on top of the metasurface. When the whole sample is heated up to a critical temperature of 58°C, the LC undergoes nematic to isotropic phase transition (Fig.9c-d). The refractive index at 1550nm changes from anisotropic one $n_o=1.51$ and $n_e=1.70$ to isotropic one $n_{iso}=1.55$. The experimental results show that the electric resonant mode shows blueshifts by 40nm and transmission contrast is up to 500% at near-infrared frequencies (Fig.9e). The phase transition of LC could also be enabled by electric field. Komar et al. demonstrated an active control of both electric and magnetic dipole modes in silicon metasurface covered by 5 μ m LC⁸³. Applying the electric field across the LC film reorients the LC molecules, thus causing the refractive index change. From Fig.9f-g, it can be

found that resonant tuning is as large as 50nm and simultaneously transmission change is up to 70% at around 1550nm while the applied AC bias voltage is 70V at 1kHz. The electric tuning effect can be further amplified if the LC is integrated into a silicon metasurface that supports high-Q modes. Parry et al. experimentally demonstrated that by applying the bias gating on the LC tuning wavelength range is more than three resonance widths for the high-Q mode ($Q \approx 270 \pm 30$)⁸⁴. In addition to resonance tuning, Li et al. combined LC with Huygens TiO₂ metasurface to realize a spatial light modulator⁸⁵ with a pixel size $\sim 1\mu\text{m}$. Such a spatial light modulator operates with a measured efficiency of 36% and a deflection angle of 11° . Transition conductive oxides, such as indium tin oxide (ITO) and aluminium-doped zinc oxide, have emerged as new materials for nanophotonics because epsilon near zero modes can be achieved by applying bias voltages. Although the penetrating depth is only several nm, large modulating depth on the reflection or transmission amplitude is still possible when the ITO is coated on the resonant photonic structures. For example, Kim et al. demonstrated that the reflection amplitude at resonance can be electrically tuned from 4% to 86% for ITO-coated silicon metagrating that supports high-Q leaky mode resonance⁸⁶. Through harnessing the epsilon near zero mode in ITO and Huygens all-dielectric metasurface, Howes et al. experimentally realized the dynamic control on the transmission amplitude⁸⁷ with modulation depth up to 31%.

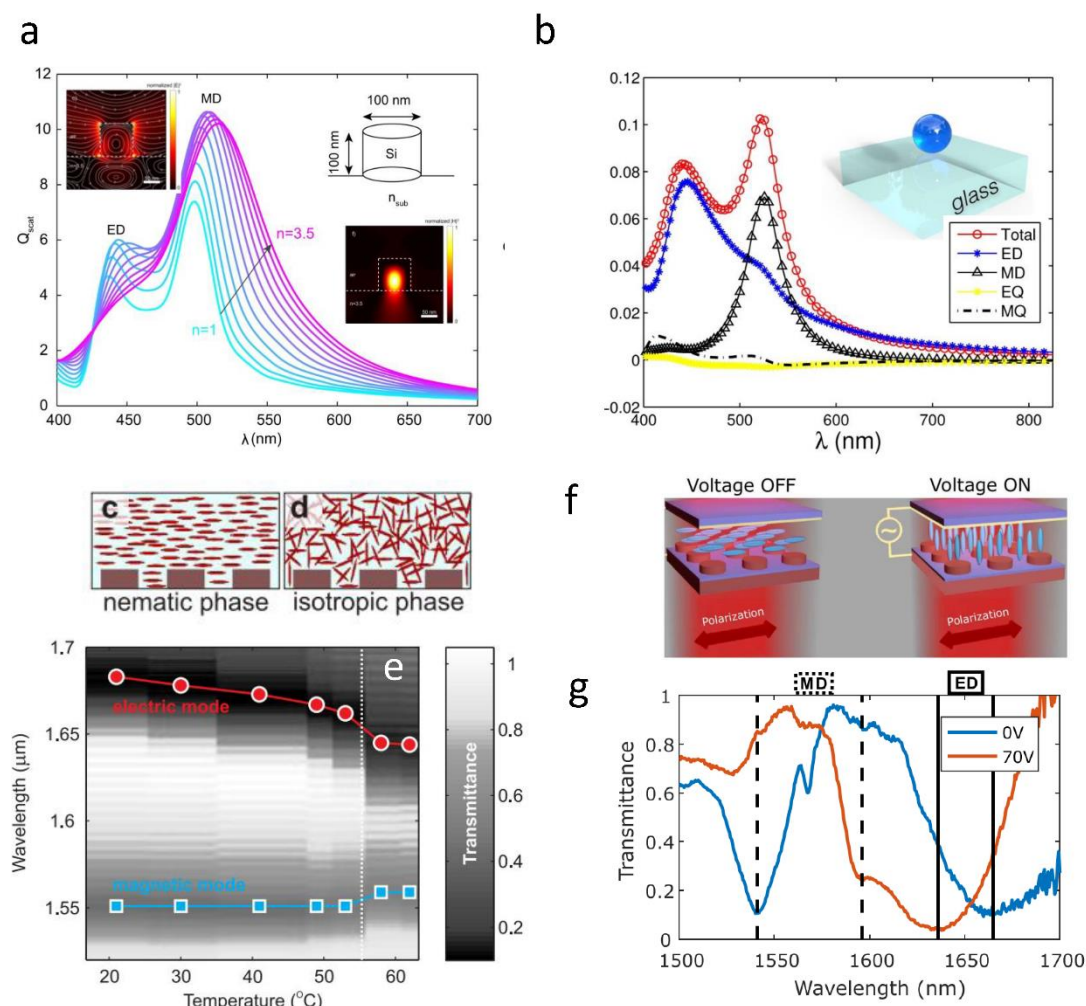


Fig.9. Mode engineering by substrate and superstrate. (a) scattering efficiency of a single Si cylinder on a semi-infinite substrate with different refractive index. Inset shows the schematic drawing of Si cylinder, electric field and magnetic field distribution of magnetic dipole mode. (b) Multipolar analysis of the extinction

cross-section of Si nanosphere on the top of glass substrate. (c-d) Schematics of LC molecules in nematic phase and isotropic phase. (e) Temperature-controlled transmission spectra of the Si metasurface capped by LC. (f) Schematic of LC molecules without and with applied voltage. (g) Measured transmission spectrum of the metasurface for $V_b=0V$ and $V_b=70V$. (a) from Ref ⁷⁹. (b) from Ref ⁸¹. (c-e) from Ref ⁸². (f-g) from Ref ⁸³.

2.3.3 Mode Engineering by Thermal, Optical, and Mechanical Tuning

Thermal tuning

As demonstrated in section 2.2, the eigenvalues of the leaky modes strongly depend on their refractive index for a given dielectric nanostructure. This suggests that one could actively tune the leaky modes' properties (e.g. resonant frequency and Q-factor) by changing the refractive index of nanostructures. Heating has been proven as an effective way of modulating the refractive index.

As the most abundant material on the earth, silicon has a temperature-dependent refractive index. Thus, it has been widely used to finely tune the resonance of silicon ring resonators. In 2017, Rahmani et al. successfully demonstrated active and reversible tuning of the Mie resonance at near-infrared wavelength range⁸⁸. Experimental results indicate that all resonances within the spectrum of interest show redshift by 30nm when the temperature increases from 20°C to 300°C. Moreover, a large forward-to-backward scattering ratio has been demonstrated, signifying that the heating may effectively control radiation directionality. Meanwhile, Lewi et al. realized large tunability⁸⁹ by several linewidths for high-Q Mie resonance of a single PbTe nanosphere and nanocuboid in the Mid-infrared window even when the temperature variation is $\Delta T \sim 10K$ (Fig.10a). Such an exceptional tunability mainly originates from the increasing thermal-optical coefficient at low temperature and high-refractive index ($n \sim 6$). Except for PbTe, researchers from the same group developed a tunable Mie resonator⁹⁰ with intrinsic InSb nanoantenna on heavily doped InSb. The fundamental physics behind it is rooted in the free-carrier generation due to the heating process. Such a thermal free-carrier production induces a positive refractive index shift ($\Delta n > 1.5$) for doped InSb but a negative refractive index shift ($\Delta n \sim -1$), both of which are almost one-order of magnitude larger than the conventional thermal-optics materials. Moreover, it is worth noting that the thermal free-carrier generation enables the realization of epsilon near zero materials for heavily doped InSb. The combination of intrinsic InSb Mie resonator and heavily doped InSb substrates may provide a new route for achieving reconfigurable photonic devices in the mid-infrared wavelength range.

Besides the thermal-optical materials, phase-changed materials (PCM) have also been widely used to control the optical properties of PCM-based nanoresonators⁹¹. When the temperature increases above a critical value, PCM experiences the amorphous-to-crystalline transition, giving rise to the effective tuning of the refractive index. Among these PMCs, $Ge_2Sb_2Te_5$ (GST) received particular attention because it has a high-index but relatively low dissipation loss in the near-infrared regime. Moreover, the transition from amorphous-to-crystalline is non-volatile. Therefore, the process is reversible. Given so many salient properties, GST has been widely utilized to develop the active dielectric metasurface with different functionalities. For example, by harnessing the drastic change of optical properties, Tian et al. experimentally demonstrated the dynamic control of multipolar Mie resonances in GST NP in the mid-infrared⁹². The continuous tuning on the refractive index during the heating process allows for the transition from electric dipole resonance to anapole state in a broadband wavelength range ($\Delta\lambda/\lambda \sim 15\%$). In addition to heating PCMs, phase transition also could be induced by a laser pulse. Through leveraging the high-Q resonance in a subwavelength GST grating, Karvounis et al. realized a large switching-ratio in reflection spectrum⁹³ when GST experiences amorphous-to-crystalline transition.

Note that above demonstrated devices are limited in thermal tuning. Recently, two research groups independently demonstrated that phase changed material-based metasurface could be tuned in both electrical and thermal way^{94,95}, bringing much more freedom of modulating the light scattering or reflection (Fig.10b-c).

Optical tuning

High-intensity laser irradiation also can modify the real (or imaginary) part of the refractive index of semiconductors by inducing free carrier generation. Although the magnitude change is very small compared to thermal-optical effects, considerable resonant shift still can be observed when a high index Mie resonator is illuminated by laser pulse. By taking advantage of localized magnetic Mie resonance in an amorphous Si nanodisk array, Shcherbakov et al. realized ultrafast all-optical switching with an ultrafast laser pulse⁹⁶ (Fig.10d). Experimental results indicate that the modulation depth is up to 60%, and the resonance shift is 6nm when the structure is pumped by picojoule-per-disk powers. Such a dynamic control can be attributed to the change of refractive index induced by free carrier generation in two photon-absorption processes. Similar ultrafast control has been demonstrated on the direct-bandgap semiconductor-GaAs metasurface by the same group⁹⁷. With a very low power fluence ($<400\mu\text{J}/\text{cm}^2$), the reflection modulation magnitude is up to 0.35 at MD resonance while the resonance experiences blueshift 30nm. Phototunable Si Huygens metasurface has also been demonstrated in the terahertz range⁹⁸. Under an ultralow optical pumping fluence ($10\mu\text{J}/\text{cm}^2$), Fan et al. demonstrated that such a metasurface has a modulation depth of 99.83% at 1.03THz and phase change $\phi > \pi/2$ (Fig.10e). Such a large tunability can be mainly ascribed to the photodoping induced refractive index change, which leads to the modification of magnetic-dipole-like odd mode. As a result, the mode degeneracy is lifted, and critical coupling is no longer satisfied.

Mechanical tuning

The eigenvalue of leaky modes in a dielectric metasurface can be tuned by interspacing between unit cells, which can be made by putting the metastructure on a flexible substrate like polydimethylsiloxane (PDMS). In 2015, Gutruf et al. experimentally demonstrated a mechanically tunable dielectric resonator at visible frequency⁹⁹. They found that %6 applied strain could induce leaky mode resonance redshift 5.08% and blueshift 0.96% for two different polarizations (Fig.10f-g). This is mainly caused by the stronger (weaker) lattice coupling along (perpendicular to) the applied-strain direction. By placing TiO_2 metasurface onto a PDMS substrate, Zhang et al. successfully realized a large spectrum tuning spanning from 450nm and 650nm¹⁰⁰. The excellent spectrum tunability by strain has found application in achieving a dynamic structural color, which is discussed in the following sections.

multi-dimensional potential. It is defined as the resonant states embedded into the continuum of unperturbed Hamiltonian due to coupling with the continuum, and thus has a finite lifetime. Recently, non-Hermitian photonics has gained extensive interest because it provides a fundamentally new platform for manipulating electromagnetic waves^{103–106}. The emergence of non-Hermitian photonics could be traced back to a pioneer work by Bender et al.¹⁰⁷, where they found that Hermiticity is not the necessary condition of realizing real eigenvalues. The real eigenvalues could also be supported in the non-Hermitian Hamiltonian when such a Hamiltonian follows PT-symmetry. Generally speaking, in photonics, non-Hermitian systems are open systems and need to interact with the exterior environment. They support many complex eigenmodes, noted as leaky modes or QNMs.

PT-symmetry and EPs

We use a simple but representative example to illustrate how Hamiltonian commuting with PT-symmetry can lead to a real eigenvalue in the spectrum. Let us consider a two-level system (Fig.11a), in which two leaky modes are coupled to each other. Its Hamiltonian takes the following form

$$H = \begin{pmatrix} \omega_1 - i\gamma_1 & \kappa \\ \kappa & \omega_2 - i\gamma_2 \end{pmatrix} \quad (19)$$

where ω_1 and ω_2 are respectively the resonant frequencies of the two modes, and γ_1 and γ_2 are radiative decay rates of two modes. κ corresponds to the coupling strength of two modes. Note that κ is not limited to a real value, but could be extended to be complex. It is easy to observe from Eq. (19) that the Hamiltonian is non-Hermitian matrix because of $H \neq H^\dagger$. Then, the eigenvalues of Eq.(19) could be obtained as,

$$\omega_{\pm} = \frac{(\omega_1 + \omega_2)}{2} - \frac{(\gamma_1 + \gamma_2)}{2}i \pm \sqrt{\kappa^2 + \Gamma^2} \quad (20a)$$

$$\Gamma = \frac{(\omega_1 - \omega_2)}{2} + \frac{(\gamma_1 - \gamma_2)}{2}i \quad (20b)$$

When $\kappa^2 + \Gamma^2 = 0$, both eigenvalues and eigenvectors become coalesced. This is called an EP. At EP, the Hamiltonian could not be diagonalizable. The EP could be realized in two special cases: (1) If the coupling strength κ is purely real, EP happens only at $\omega_1 = \omega_2$ and $\kappa = \frac{(\gamma_1 - \gamma_2)}{2}$. (2) If the coupling

strength κ is pure imaginary, EP could be reached at $\gamma_1 = \gamma_2$ and $\kappa = \frac{(\omega_1 - \omega_2)}{2}i$. From the

mathematic point of view, EP is a singularity point and could be accessed by sweeping two parameters

(i.e., coupling strength κ and resonant frequency difference $\omega_d = \frac{(\omega_1 - \omega_2)}{2}$), as highlighted in

Fig.11b-c. In fact, EP is also the transition point between strong coupling and weak coupling. In the strong coupling regime $\kappa > \kappa_{EP}$, the real part of the eigenvalue shows anti-crossing behavior while the imaginary part crosses. In the weak coupling regime $\kappa < \kappa_{EP}$, opposite phenomenon occurs at zero detuning point. At transition point $\kappa = \kappa_{EP}$, both real and imaginary parts of two eigenvalues kiss each other at zero detuning point $\omega_d = 0$.

Note that the eigenvalues could become real if $\gamma_1 = -\gamma_2 = \gamma$ and $\kappa^2 + \Gamma^2 \geq 0$. Assuming a real coupling strength κ , if $\omega_1 = \omega_2 = \omega_0$, then both the eigenvalues are real for $\kappa \geq \gamma$. Under this circumstance, the Hamiltonian could be further simplified as

$$H = \begin{pmatrix} \omega_0 - i\gamma & \kappa \\ \kappa & \omega_0 + i\gamma \end{pmatrix} \quad (21)$$

This Hamiltonian is PT-symmetric as it commutes with the PT operator, where parity operator P corresponds to the Pauli operator $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ while the time-reversal operator T means the complex conjugation. The rigorous proof is given in Appendix-B. A balanced gain and loss medium must be introduced to induce an equal amount of radiative decay rate with the opposite sign (Fig.11d). PT-symmetric phase is broken at $\kappa = \gamma$, which is also the occurrence of EP. When the coupling crosses the EP, the real eigenvalue evolves into a complex eigenvalue. Before transition $\kappa < \kappa_{EP}$ (PT-symmetric broken phase), the real parts of the eigenvalue show splitting while the imaginary parts remain constant at zero (Fig.11e). After passing through EP $\kappa > \kappa_{EP}$ (PT-symmetric phase), the real parts are reduced to the same value but the imaginary parts are split into two with different linewidth (Fig.11f). Here, we would like to point out that there is a subtle connection between a non-Hermitian system that only involves loss and a non-Hermitian system based on PT-symmetry that involves gain and loss simultaneously. Let us again consider a two-level system with Hamiltonian having the following form

$$H = \begin{pmatrix} \omega_0 - i\gamma_1 & \kappa \\ \kappa & \omega_0 - i\gamma_2 \end{pmatrix} = \begin{pmatrix} \omega_0 - i\beta & \kappa \\ \kappa & \omega_0 + i\beta \end{pmatrix} + \begin{pmatrix} -i\alpha & 0 \\ 0 & -i\alpha \end{pmatrix} \quad (22)$$

Where $\alpha = (\gamma_1 + \gamma_2)/2$ and $\beta = (\gamma_1 - \gamma_2)/2$. The first matrix on the right could be viewed as a new Hamiltonian satisfying PT-symmetry, and the second matrix represents the lossy terms. From Eq.(22), it can be inferred that a non-Hermitian system only involving loss can be treated as a passive PT-symmetry system. From a fundamental physics perspective, the physical nature of non-hermitian photonics is leaky mode engineering via delicate control on the gain and loss in a coupled resonator system and coupling between them.

BICs and QBICs

Proper engineering of the coupling between two leaky modes could lead to the generation of BIC or QBIC in an open system. To illustrate their physical mechanisms, we again consider the two-level system with complex coupling. For the sake of generality, the off-diagonal coupling term is set as different values^{108,109}

$$H = \begin{pmatrix} \omega_1 - i\gamma_1 & \kappa_1 \\ \kappa_2 & \omega_2 - i\gamma_2 \end{pmatrix} \quad (23)$$

The eigenvalues of the matrix can be obtained by diagonalization of the matrix, and are expressed as follows

$$\omega_{\pm} = \frac{\omega_1 + \omega_2}{2} - i \frac{(\gamma_1 + \gamma_2)}{2} \pm \sqrt{\frac{[(\omega_1 - \omega_2) + i(\gamma_1 - \gamma_2)]^2}{4} + \kappa_1 \kappa_2} \quad (24)$$

The Q-factors for uncoupled and coupled modes can be obtained by

$$Q_1 = \omega_1 / 2\gamma_1, \quad Q_2 = \omega_2 / 2\gamma_2 \quad (25a)$$

$$Q_+ = \text{Re}(\omega_+) / 2\text{Im}(\omega_+), \quad Q_- = \text{Re}(\omega_-) / 2\text{Im}(\omega_-) \quad (25b)$$

When $\gamma_+ = 0$ or $\gamma_- = 0$, one of the leaky modes reduces to BIC. Now, let us consider an even simpler case to illustrate this, $\omega_1 = \omega_0, \omega_2 = \omega_0 + \Delta, \gamma_1 = \gamma_2 = \gamma_0$, where Δ is the frequency detuning. Then, Eq.(24) can be rewritten as

$$\omega_{\pm} = \omega_0 + \frac{\Delta}{2} - \gamma_0 i \pm \sqrt{\frac{\Delta^2}{4} + \kappa_1 \kappa_2} \quad (26)$$

According to Eq.(26), the imaginary parts of $\omega_{\pm}$ could be reduced to zero by properly choosing the complex coupling $\kappa_1\kappa_2$. Thus, in principle, BIC could be constructed in such a simple two-level system. A concrete example of BIC formation is shown in Fig.11g-h, where $\omega_0 = 2$, $\gamma_0 = 0.01$, and $\kappa_1\kappa_2 = 2.0 \times 10^{-4}i$. Interestingly, the real parts of eigenvalue $E_{\pm}$ display anticrossing at $\Delta = 0$ and simultaneously one of the imaginary parts is suppressed to zero while the other is enhanced to the maximum. When $\kappa_1\kappa_2$ deviates from this critical value, the imaginary part becomes nonzero, as shown in Fig.11i, indicating the transition from BIC to QBIC. Note that BIC or QBIC can also be constructed in the case of eigenvalue crossing. In fact, this type of BIC, called as Friedrich-Wintgen BIC, has already been studied in quantum mechanics¹¹⁰ and acoustics^{111,112} due to resonance interference in different channels. Thus, building crossing or avoided crossing is a universal rule of realizing BIC or QBIC in single or multi NPs, which are discussed in section III.

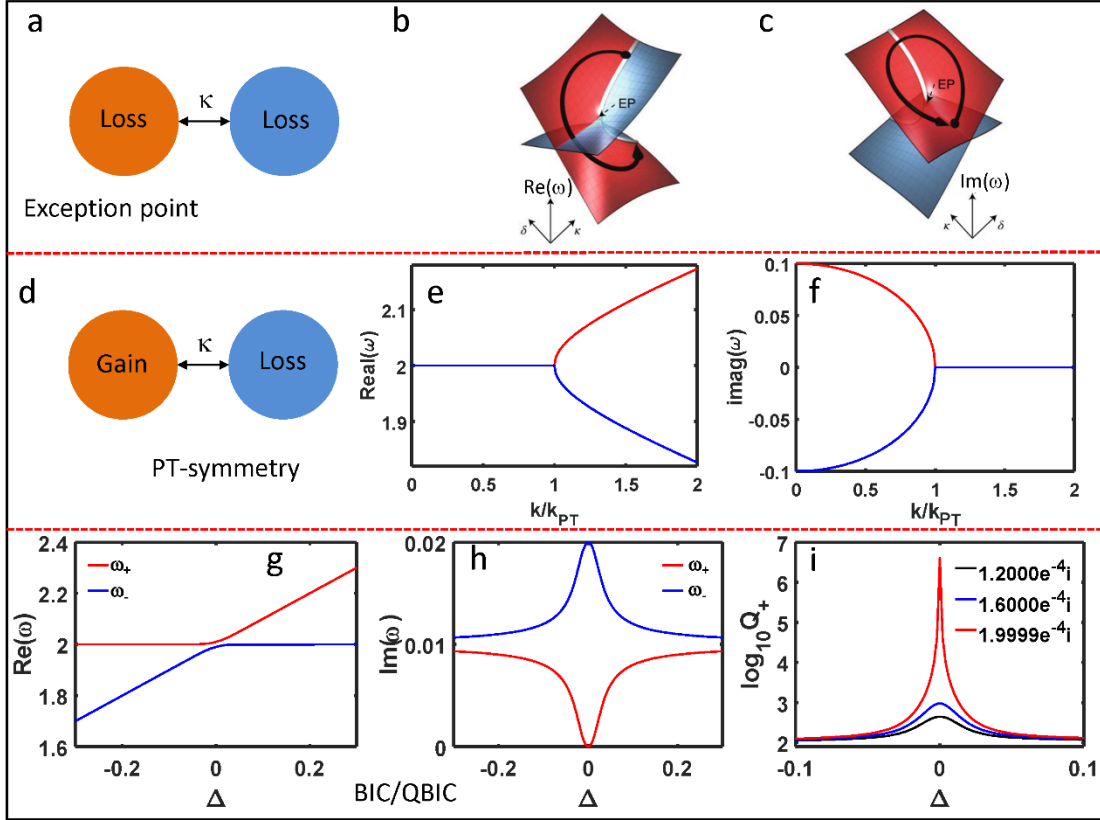


Fig.11. Leaky mode engineering by non-Hermitian coupling. (a) Schematics of two coupled lossy resonators. (b-c) 3D contour plot of real and imaginary parts of complex eigenfrequency. (d) Schematics of coupled resonators with balanced gain and loss. (e-f) Real and imaginary parts of complex eigenfrequencies as a function of coupling strength. (g-h) Real and imaginary parts of complex eigenfrequencies vs detuning frequency. (i) Q-factors of high-Q mode vs varied coupling strength. (b-c) from Ref¹⁰⁶.

2.4. Application of leaky modes in light-matter interaction

2.4.1 Perfect Absorber

One of the most appealing applications for leaky modes is perfect light absorbers^{113,114}. When a plane wave impinges on a lossy medium, perfect absorption can be achieved through careful engineering of the structure parameters and judicious choice of material parameters. As early as 1936, theoretical and experimental work found that a quarter wavelength resonant absorber with carbon black, and titanium dioxide for reduced thickness, could be used for antennas operating at 2 GHz to improve the front-to-back ratio¹¹⁵. However, much more significant interest in electromagnetic absorbers began during World War II, due to the high attenuation of radar possible with such absorbers, which enabled military advantages¹¹⁶.

The emergence of metamaterials brought about unprecedented freedom in manipulating the propagation and attenuation of electromagnetic waves. Landy et al. proposed a pioneering design of a perfect absorber in the microwave range based on metamaterials consisting of an array of metallic split ring resonators and cut wires¹¹⁷. Later, numerous studies were conducted to push the operation wavelength of metamaterial-based perfect absorbers to terahertz¹¹⁷, near-infrared^{118,119} and visible¹²⁰ wavelength ranges. The most frequently used design is an array of metallic structures (i.e., split ring resonator, gold NPs) sitting on a dielectric layer backed by a continuous metal film. Although metamaterial-based absorbers have found many applications, such as optical sensors¹¹⁸ and thermal emitters¹²¹, they possess some fundamental limitations because many designs utilize metals. In most studies, the absorbed energy is converted to heat, although energy harvesting¹²² and detector designs are an exception¹²³. In other studies, metamaterial absorbers are used as emitters, and it is desirable to operate them at high temperatures due to the T^4 dependence of the Stefan-Boltzmann law. Thus the relatively low melting temperature of metals limits their applications in thermophotovoltaics, controlled incandescence, and other applications which require high operating temperatures ($T > 1000^\circ$). This issue is partially mitigated by using refractory materials like TiN¹²⁴. However, metals and refractory materials possess poor electrical conductivity, and are not compatible with CMOS technology. Thus, more recently researchers and scientists have performed studies on all-dielectric perfect absorbers based on semiconductors^{125,126} and ceramics³⁹, due to their potential high-temperature operation, lack of Ohmic loss, and relatively low thermal conductivity.

Section 2.1 has demonstrated that the maximum absorption contributed by a single resonance is 50% for single-side illumination when the critical coupling condition is satisfied. Thus, through the addition of a second resonance of opposite symmetry – odd in this case – perfect absorption can be realized. For example, Pieper et al. used TMCT and simulations to show unity light absorption with monolayer graphene by placing it onto a silicon photonic crystal slab backed with a PEC mirror or distributed-Bragg-reflector-based mirror³⁷, as shown in Fig.12a-b. In another study, Liu et al. experimentally verified that such a design achieves 85% absorption at 1545.5nm.¹²⁷ Previous studies also used a metal-backed resonator to utilize two resonances of opposite symmetry to achieve perfect absorption, with the first well-known study at terahertz frequencies¹²⁸. Since this design strategy is universal and robust, it has been generalized to design perfect absorbers in many other wavelength regimes. For example, Huang et al. found that three layers of MoS₂ ($t \approx 2\text{nm}$) could absorb more than 70% of incident light¹²⁹ when they were transferred on top of the GaN metagrating with a back mirror coating behind the sapphire substrate, as shown in Fig.12c.

As mentioned, in addition to the single port two modes of opposite symmetry strategy, it is also possible to achieve perfect absorption with degenerate modes satisfying critical coupling simultaneously¹³⁰. Before discussing the specific design that supports degenerate modes, it is necessary

to illustrate the fundamental physics behind it. For a free-standing semiconductor film with intrinsic loss, one-side illumination with E_x polarization could be viewed as the superposition of two coherent sources³⁸ (See Fig.12d), which is expressed as follows

$$E_{inc} = (E_{up}, E_{down}) = (E_0, 0) = \left(\frac{E_0}{2}, \frac{E_0}{2}\right) + \left(\frac{E_0}{2}, -\frac{E_0}{2}\right) = E_{even} + E_{odd} \quad (27)$$

A leaky mode always has either a symmetric or antisymmetric distribution with respect to the central mirror plane, either an in-phase or out-of-phase coherent source can be absorbed, and therefore a maximum absorption of 50% is possible from a single resonance. Assuming that the system supports two leaky modes, where one is an even mode and the other is an odd mode, the total absorption contributed by two modes can be obtained by simply summing up their individual contributions,

$$A = \frac{2\gamma_0\gamma_{even}}{(\omega_{even}-\omega)^2+(\gamma_0+\gamma_{even})^2} + \frac{2\gamma_0\gamma_{odd}}{(\omega_{odd}-\omega)^2+(\gamma_0+\gamma_{odd})^2} \quad (28)$$

Thus Eq. (28) shows that the total absorption can be 100% only when $\gamma_{even} = \gamma_{odd} = \gamma_0$, $\omega_{even} = \omega_{odd}$. In other words, complete absorption is achieved when two degenerate resonances with opposite symmetry satisfy critical coupling at the same time. Using the temporal CMT description of the absorption process, Piper et al. presented a theoretical prediction of unity absorption¹³⁰ at near-infrared wavelength range in a hybrid system consisting of monolayer graphene on top of a silicon photonic crystal slab, which satisfies degenerate critical coupling. Liu et al. experimentally verified this strategy by showing a 100% absorption¹²⁶ at 1.01THz in a dielectric metasurface whose unit cell is a silicon cylinder, as shown in Fig.12e-f. Such a metasurface supports electric and magnetic dipole resonances, which are degenerate but with opposite symmetry. Ming et al. revealed that this perfect absorber is indeed induced by the degenerate critical coupling³⁸. In fact, if the system is lossless, a Huygens metasurface could be fashioned. Tuning the intrinsic loss to achieve critical coupling converts the metasurface from a Huygens metasurface to a perfect absorber¹³¹. There are also many other designs capable of achieving perfect absorption based on the degenerate critical coupling description^{132–135}. It is important to stress, that the degenerate critical coupling strategy for perfect absorption only works at normal incidence. This strict requirement could be removed by considering a structure with inverse symmetry. Zhou et al. reported the perfect absorption in a single-sided illumination¹³⁶.

Coherent perfect absorption (CPA) uses a single even or odd symmetry resonance to achieve absorption, and may be viewed as time-reversed lasing¹³⁷ (See Fig.12g). To explain the operation principle of CPA, it is necessary to introduce the concept of scattering poles and scattering zeros¹³⁸. For simplicity, we consider a single slab layer that may be illuminated from both sides. The scattering matrix for such a system can be expressed as follows

$$S = \begin{pmatrix} r_{11} & t_{21} \\ t_{12} & r_{22} \end{pmatrix} \quad (29)$$

where $r_{11}(t_{12})$ and $r_{22}(t_{21})$ represent the reflection (transmission) coefficients under left and right illumination, respectively. There are a series of scattering zeros and scattering poles for such a scattering matrix. Section 2.1 shows that scattering poles correspond to the leaky modes. For a system involving no gain or loss, the scattering matrix S must be unitary, meaning $SS^+ = I$. Also, the scattering zeros and scattering poles are complex conjugates to each other. More specifically, the eigenvalue for scattering zeros has positive real and imaginary parts, while the eigenvalue for scattering poles has positive real parts but negative imaginary parts. Upon adding loss to the dielectric slab, the scattering poles move toward zero. The CPA condition occurs only when the scattering pole touches zero on the real axis, as shown in Fig.12h. An experimental demonstration was conducted by Wan et al.

in 2011¹³⁹. Through manipulation of the relative phase of two beams, the absorption of a silicon wafer could be tuned between 0 and 100%, as demonstrated in Fig.12i. CPAs were also proposed theoretically and demonstrated experimentally with various designs based on metamaterials^{140–142}. Here, it is worth noting that the perfect absorber discussed above operates at a single wavelength, and broadband absorbers are discussed in the solar cell section.

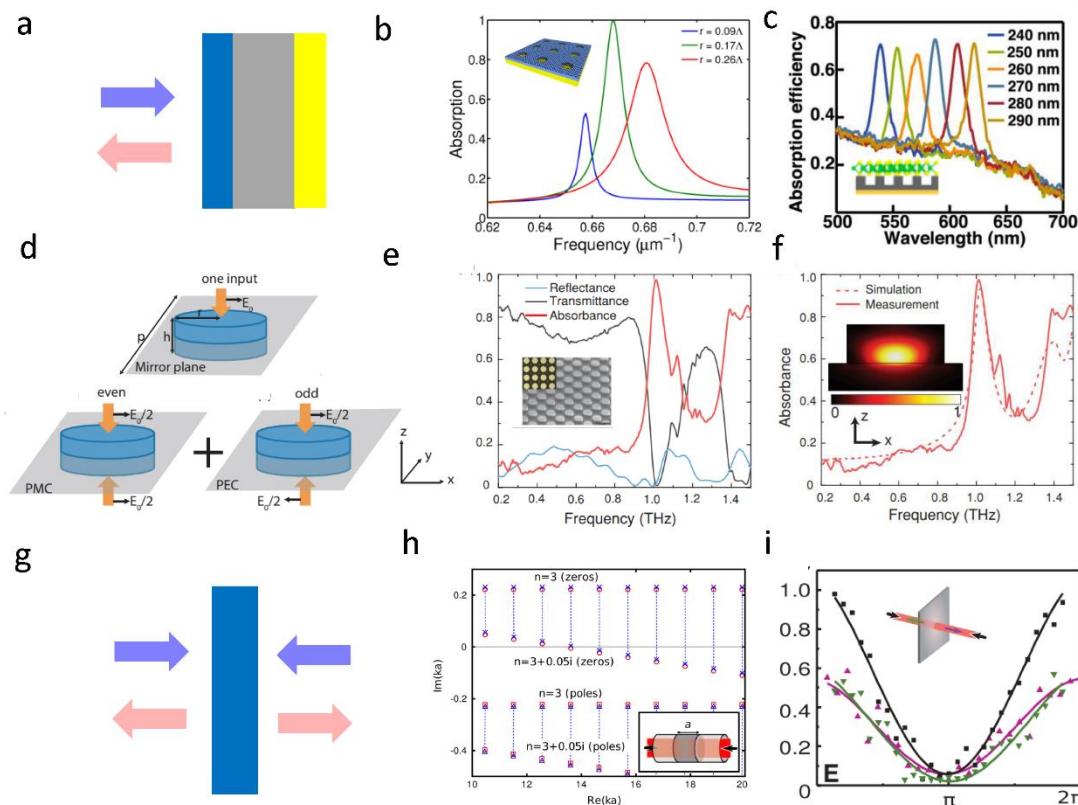


Fig.12. Perfect absorber and coherent perfect absorber. (a) Schematic drawing of perfect absorber based on single-port system with mirror. (b) The absorption spectrum of monolayer graphene sitting on a photonic crystal slab backed by a mirror at three different hole radii $r=0.09\lambda$, $r=0.17\lambda$, $r=0.26\lambda$. (c) Measured absorption spectrum of three-layer MoS₂ on GaN metagrating with Ag coating behind the substrate. (d) Schematics of perfect absorber based on degenerate critical coupling. (e) Measured reflection, transmittance, and absorption spectra in a silicon metasurface. (f) Comparison of simulated and measured absorption spectrum. The inset is the electric field distribution at perfect absorption wavelength. (g) Schematic of coherent perfect absorber. (h) Scattering zeros and scattering poles in the complex frequency plane. (i) Absorption of silicon slab versus the relative phase of two coherent-illumination beams from both-sides. (b) from Ref ³⁷. (c) from Ref ¹²⁹. (d) from Ref ³⁸. (e-f) from Ref ¹²⁶. (h) from Ref ¹³⁷. (i) from Ref ¹³⁹.

2.4.2 Solar cell and photodetector

Leaky mode engineering plays a central role in enhancing the performance of many photonic and optoelectronic devices. The most representative examples are solar cells and photodetectors. This section reviews the recent progress in developing the high-performance solar cells and photodetectors by judiciously engineering the leaky modes¹³.

Enhanced solar absorption by leaky modes

The key to designing high-performance solar cells is to have strong light absorption in the solar spectrum. One of the most abundantly used semiconductor materials for a solar cell is silicon. However, the mismatched impedance between silicon and air creates the undesired reflection, significantly degrading solar cells' performance. Spinelli et al. found that the reflection happening at the interface of silicon wafer and air could be almost eliminated across a broadband range of 450nm-900nm by creating an array of low aspect-ratio Si nanocylinders¹⁴³. The fundamental physics behind this interesting phenomenon is that leaky mode resonance supported by Si nanocylinder array strongly couples to the substrates, leading to the destructive interference that suppresses the reflection. This suggests the Mie resonator array could serve as an effective antireflection coating layer. Numerical calculation shows that the solar cell efficiency is increased to 21.5% for 20 μ m Si solar cell by patterning a silicon nanocylinder array as an antireflection coating layer¹⁴⁴.

Wang et al. derived a rigorous condition of realizing perfect antireflection coating with a leaky mode resonance based on temporal CMT⁴². On the one hand, the periodicity of the array should fall within the subwavelength scale to eliminate the high-order diffraction so that only zero-order diffraction dominates. On the other hand, a delicate balance should be reached between radiation into substrate and radiation into air. Later, multi-resonant silicon metasurfaces by either harnessing compound unit cell¹⁴⁵ or combing Fabry-Perot and Mie resonances¹⁴⁶ have been proposed to further improve the performance of antireflection coating layer. The significantly reduced reflection in broadband range could contribute to the enhanced broadband absorption, as experimentally demonstrated in many works^{147,148}. For example, broadband light absorption could be achieved by using a metasurface that supports multi-resonances. Kim et al. successfully realized a strong broadband absorption with a 40 nm Ge metafilm sitting on the gold substrate¹⁴⁹, whose unit cell is made of several nanobeams of different size. Each nanobeam array supports a low-Q leaky mode, and thus contributes to enhanced absorption. Combining several nanobeams array directly leads to broadband absorption.

According to the temporal CMT described in section 2.1.2, optical resonance plays a vital role in boosting light absorption. Thus, many groups have devoted numerous efforts to promote light absorption by judiciously designing solar cells with resonant photonic structures. Cao et al. demonstrated that semiconductor NW optical antennas could efficiently absorb solar light by capitalizing their leaky modes¹⁵⁰. Grandier et al. placed an array of wavelength scale dielectric nanosphere on the top of a thin-film solar cell to enhance their light absorption and photocurrent because it supports whisper gallery modes at interest wavelength range¹⁵¹. Besides, Yao et al. found that even a monolayer of 50nm nanocrystalline silicon nanoshell enabled a broadband strong light absorption across a wide range of incident angles (Fig.13a-d), comparable to the absorption of micrometre silicon¹⁵². The superior performance of this structure is attributed to the low-Q whisper gallery mode. Ferry et al. presented a comprehensive study on light trapping in amorphous-silicon-based thin-film solar cell¹⁵³, which clarified the role of metal contact and patterned semiconductors in absorption enhancement. The theoretical analysis facilitates the optimization of the solar cell.

Except for this specific photonic structure design, there are also numerous efforts on studying the theoretical limit of light trapping enabled by resonant nanophotonic structure. For conventional solar cell whose thickness is a few wavelengths, there is an upper limit of absorption enhancement factor $4n^2/\sin^2\theta$ according to the light trapping theory. The operation principle behind it lies in the total internal reflection between high-index semiconductors and low-index surrounding medium. When the

absorption layer thickness is comparable to or even smaller than the wavelength, the conventional limit does not hold any more. The proper nanophotonic design could help to overcome this limit^{154,155}. Yu et al. tackled this issue by developing a statistic coupled-mode theory¹⁵⁴, where over-coupling instead of critical coupling has been used to maximize the absorption enhancement in a broadband manner. Numerical simulations show that the absorption enhancement factor can approach $12 \times 4n^2$ by exploring the subwavelength modal confinement. Yu et al. also explored the light-trapping scheme of multilayer thin-film solar cells based on temporal CMT and found that even 10nm amorphous silicon could absorb majority of sunlight¹⁵⁶. High-efficiency broadband light trapping, which approaches the theoretical limit, has been experimentally demonstrated in thin-film solar cells by employing quasi-random nanostructures made of binary grating¹⁵⁷.

Photodetector

Similar to the solar cell, strong light absorption is required to achieve a high-performance photodetector. Taking the photodiode as an example, the incident photon above the bandgap of the semiconductor is first absorbed to excite electrons from the valence band to the conduction band, leaving a hole in the valence band. When a reverse bias is applied, generated electron-hole pair will drift out of the semiconductor and form the photocurrent. Thus, it is always desirable to have unity light absorption at the operation wavelength of a photodetector. Previous section has indicated that absorption efficiency could be greatly enhanced by an optical resonance. Proper engineering of optical resonance can help to improve the performance of photodetectors. Cao et al. reported a polarization-sensitive near-infrared photodetector based on a single Ge NW¹⁵⁸. The diameter of NW is carefully tuned to support a leaky mode resonance at telecommunication. Thanks to the leaky modes, the photoresponse shows 25 folds enhancement compared to the thin film with the same thickness. In 2019, Siday et al. demonstrated a GaAs-based photoconductive metasurface that could perfectly absorb the incident light¹³⁵ (Fig.13e-f). The unit cell consists of a cuboid and a long-side nanobar. Thus, the whole metasurface also could serve as an electrically connected network. The unity absorption is enabled by the degenerate modes with opposite symmetry that satisfy the critical coupling simultaneously. The metasurface could switch from resistive (off) state to conductive (on) state by using an ultralow optical pumping power with an ultrahigh on/off ratio $>10^7$ (Fig.13g). In addition, the authors demonstrated terahertz (THz) pulse detection by integrating the perfect absorbing metasurface with THz antenna, whose signal to noise ratio is more than six orders of magnitude under an ultralow level of laser excitation (Fig.13h).

Except for photodetection at a single wavelength, a multiwavelength photodetector has also been developed based on an all-dielectric metasurface. By leveraging the anti-Hermitian coupling, Kim et al. realized a photo-sorting photodetector with near-unity sorting efficiency and near-unity absorption¹⁵⁹. The spectral separation of sorted photons is $\sim 30\text{nm}$. Another example is the transparent multispectral photodetector proposed by Li et al.¹⁶⁰ (Fig.13i). It is built upon a silicon NW array that provides degenerate resonances with opposite symmetry with respect to the central mirror plane of the array (Fig.13j), which not only cancel the backward scattering but also boost the light absorption at a different wavelength. Such a photodetector allows for the simultaneous detection of light intensity, polarization, and color (Fig.13k-l). Recently, an angle-sensitive photodetector was developed by exploiting the non-Hermitian coupling of two closed-packed subwavelength silicon NW¹⁶¹. The angle sensitivity is as low as 0.32° .

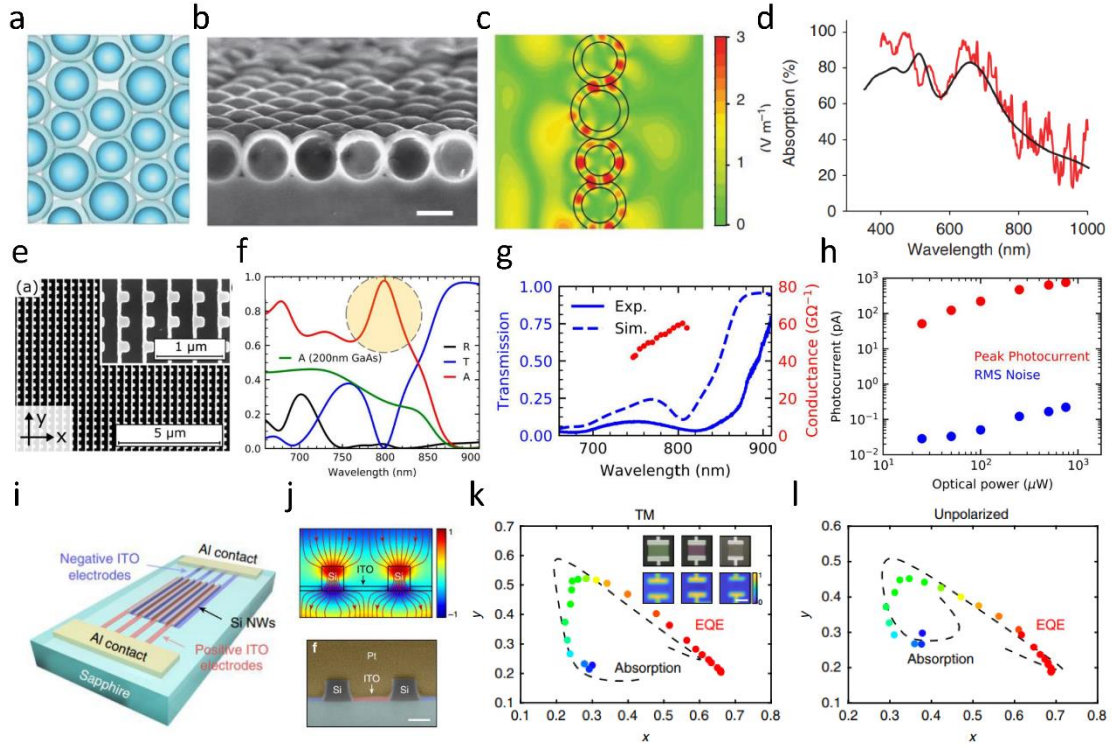


Fig.13. Solar cells and photodetectors enabled by leaky mode engineering. (a) Schematic drawing of Si spherical nanoshell array with different sizes. (b) SEM image of Si nanoshell array. (c) Electric field distribution of leaky mode resonance. (d) Measured and simulated absorption spectrum. (e) SEM image of a GaAs metasurface. (f) Simulated reflection/transmission/absorption spectra of GaAs metasurface. (g) Comparison of measured and simulated transmission spectra and photoconductive spectra. (h) Peak photocurrent and RMS noise versus optical pumping power. (i) Schematic drawing of multispectral photodetector. (j) Top panel is electric field distribution at leaky modes resonance for the Si/ITO-based photodetector. The bottom panel is SEM image of fabricated photodetector. (k-l) CIE color plot for TM polarized and unpolarized light illumination. (a-d) from Ref ¹⁵². (e-h) from Ref ¹³⁵. (i-l) from Ref ¹⁶⁰.

2.4.3 Enhanced Light Emission and Strong Coupling

When quantum emitters are embedded into the photonic nanocavity environment, their spontaneous emission could be significantly improved via Purcell effects. The magnitude of enhancement is evaluated by the Purcell factor. For an open plasmonic or dielectric resonator, the Purcell factor has the following form^{60,162}

$$F = \frac{3}{4\pi^2} \left(\frac{\lambda_0}{n} \right)^3 \text{Re} \left(\frac{Q}{V} \right) \quad (30a)$$

$$V = \frac{\int [\mathbf{E} \cdot \frac{\partial(\omega\epsilon)}{\partial\omega} \mathbf{E} - \mathbf{H} \cdot \frac{\partial(\omega\mu)}{\partial\omega} \mathbf{H}] d^3\mathbf{r}}{2\epsilon_0 n^2 [\mathbf{E}(\mathbf{r}_0) \cdot \mathbf{u}]^2} \quad (30b)$$

Eq. (30) indicates that the Purcell factor strongly depends on the Q-factor of the cavity mode and complex mode volume. Different kinds of photonic nanocavity have been proposed to boost light

emission, and even realize lasing. One of the typical examples is plasmonic cavity made from noble metallic NPs. The most salient property of plasmonic resonance is that it enables extreme field confinement at the surface of NPs below the diffraction limits. If the dipolar emitter is put on top of the metallic NPs or located within the gap of plasmonic dimer, a huge enhancement of emission intensity is obtained.

Nevertheless, the high-loss nature of noble metals brings about non-negligible heat generations that may degrade the plasmonic-based devices' performance. As subwavelength high-index semiconductor with low loss also supports the leaky mode resonances with electric and magnetic characteristics, it may provide another effective way of engineering the light emission. In this section, we will review the applications of leaky mode resonance (or Mie-resonance) in enhancing light emission and strong coupling, which covers both the conventional materials (i.e. organic molecules, etc.) and novel materials such as two-dimensional (2D) transition metal dichalcogenide monolayer and perovskites.

Enhanced light emission

As the basic unit of the all-dielectric metasurface, an isolated high-index Mie resonator provides an excellent platform to study light-matter interaction. On the one hand, both electric and magnetic resonances allow for confining the electric (or magnetic) field within and around the nanostructures. Bringing an emitter close to the single dielectric nanoantenna could manipulate the radiation intensity. On the other hand, the rich multipolar interferences provide much more flexibility in controlling the emission directionality than plasmonic nanoantennas. Particularly, Schmidt et al. derived the decay rate of enhancement of electric and magnetic dipolar emitters when they are placed in the vicinity of spherical NP¹⁶³. They found that the enhancement factor varies with the location and polarization of the emitter with respect to the dielectric NP. Later, Zambrana-Puyalto et al. presented a theoretical investigation on the Purcell factor of multipolar mode for spherical Mie resonator¹⁶⁴. Typically, the Purcell factor of magnetic (electric) dipole resonance is limited due to the moderate near-field enhancement when the dipolar emitter is brought to the vicinity of the dielectric antenna, as demonstrated experimentally by Bouchet et al.¹⁶⁵. Aside from the emission intensity modulation, the far-field radiation pattern can also be tailored by exploiting multipole interference. For example, Cihan et al. realized an electric-dipole dominated emission forward-to-backward ratio up to 20 by placing a silicon NW onto monolayer MoS₂/sapphire substrate¹⁶⁶. Properly choosing the radius of silicon NW can help generate highly directional emission by engineering the multipolar interferences between MoS₂ dipolar emitter and electric/magnetic dipole modes.

Similar to the hot-spot in the plasmonic dimer, ultrastrong near-field is confined within the gap between the dielectric antenna dimer¹⁶⁷. Caldarola et al. demonstrated that the hot-spot within the 20-nm gap of silicon dimer could enhance the Raman from polymer thin film or molecule emission¹⁶⁸ by a factor of 1000 and 2000, respectively. However, the molecular thermometry measurements indicate that the heating effect is 1/18 times of Au plasmonic-dimer antenna. This may elevate the operation temperature of devices and avoid the melting or reshaping of the antenna. Regmi et al. further investigated the fluorescence enhancement of a single molecule¹⁶⁹ by a silicon dimer antenna with a 20nm gap. Such a narrow gap ensures the strong near-field enhancement, resulting in 270-folds fluorescence enhancement in an ultra-small volume $\lambda^3/1800$. The semiconductor dimer antenna could also be used to enhance the light emission from 1L transition metal dichalcogenide. Through integrating atomic monolayer and bilayer WSe₂ onto GaP dimer antenna, Sortino et al. reported a giant

PL enhancement factor exceeding 10^4 compared to WSe_2 on the GaP thin film with the same thickness¹⁷⁰ (Fig.14a-c). Also, Raman scattering shows three order magnitude of enhancement. Such a large enhancement is attributed to Purcell enhancement, efficient directional emission and the large absorption at the excitation wavelength.

Note that the above discussion mainly focuses on emission enhancement by placing an emitter near the dielectric antenna. The emitter also could be embedded into the NPs. Thus, a large overlap between the emitter and maximum field is attained. The experimental results show that by embedding the Ge quantum dot inside the silicon nanodisk the emission can be boosted by 10 folds through exciting the asymmetric electric and magnetic dipole mode in a linear silicon trimer¹⁷¹. Semiconductors like Ge can serve as emission materials. Under such circumstances, a single Ge nanoresonator supporting Mie-type resonance is found to be able to improve its emission by 30-folds with respect to the Ge thin film with identical thickness¹⁷². For semiconductors with high-quantum-yield, lasing becomes possible with a single NP that supports high-order Mie modes. One of the most represented materials is lead halide perovskite. As a direct-bandgap semiconductor, it has a long carrier lifetime, low nonradiative recombination rate and large quantum-yield. These unique properties render them an excellent candidate for lasing. Tang et al. successfully demonstrated the single-mode laser with submicron perovskite spheres that supports high-Q whisper gallery mode¹⁷³ (Fig.14d-e). The threshold of CsPbX_3 laser is as low as 0.42uJ/cm^2 and the line-width is only 0.09nm , indicating that the Q-factor is up to 6100. Moreover, the lasing wavelength is continuously tuned across the entire visible window (424nm - 715nm) by changing the diameter of the sphere and halide composition (Fig.14f). Since lead perovskite has a relatively large refractive index (>2) in the visible wavelength range, a single perovskite NP supports multipolar order Mie modes. In 2018, Liu et al. succeeded in building a single-mode nanolaser¹⁷⁴ based on a CsPbBr_3 cuboid with a side length of about 400nm , smaller than the operating laser wavelength. The threshold power for one-photon and two-photon excitation is 40.2 and 374 uJ/cm^2 , respectively. The retrieved Q-factors of high-order Mie modes utilised for lasing are 2075 and 1859, respectively. In 2020, by choosing the third-order or four-order Mie modes, Tiguntseva et al. realized room temperature lasing with a single subwavelength CsPbBr_3 cube with a side length of 310nm , which is half of the diameter in the previous submicron sphere¹⁷⁵. Because of the moderate $Q\sim 14$, the threshold is almost 300uJ/cm^2 . The laser threshold can be further reduced to around 100uJ/cm^2 by exciting four-order Mie mode.

When simultaneously taking account of Mie resonance and other physical effects, such as hot-electron interband transition and Auger effect, emission intensity from single NPs could be greatly improved in a broadband wavelength range. For example, despite the ultralow quantum efficiency of silicon, by using both electric and magnetic multipolar resonance, Zhang et al. demonstrated the efficient white-light emission in a single silicon NP (feature size $\sim 200\text{nm}$) with only 40pJ laser pulse¹⁷⁶. This fantastic phenomenon is attributed to the improved quantum efficiency and enhanced absorption at the excitation wavelength. The experimental results show that quantum efficiency is increased by four to five orders of magnitude compared to bulk silicon after taking three-photon-induced photoluminescence into account. Such a giant enhancement is contributed by two major factors. One is the enlarged nonradiative life time by Auger effects that are amplified by the high-carrier-density injection via resonant exciting the electric dipole/magnetic dipole resonance. The other is the reduced radiative lifetime from $10\text{-}100\text{ns}$ to $1\text{-}10\text{ns}$ due to large electric field enhancement enabled by electric

quadrupole and magnetic quadrupole resonance. Besides, the absorption efficiency is resonantly enhanced by matching the laser excitation wavelength with the magnetic dipole resonance. The quantum efficiency can be further improved by four folds by placing the silicon NP on the Ag thin film that acts as a mirror¹⁷⁷. Consequently, the threshold for generating the white-light emission is reduced to several pJ.

Since an isolated dielectric nanostructure can be viewed as an effective dielectric antenna, an all-dielectric metasurface is equivalent to an array of subwavelength dielectric antennas. It inherits the intrinsic property of a single high-index NP, supporting both electric and magnetic resonance. Except for the dimension of NP, the periodicity provides additional freedom to manipulate the Mie resonance, allowing for tailoring the near-field distribution and far-field radiation pattern. The first experimental demonstration of enhanced PbS QD emission by silicon metasurface was done by Staude et al.¹⁷⁸. When the electric and magnetic dipole resonance overlap in the spectrum, a single PL emission maximum occurs. Active control on the spontaneous emission was also demonstrated by incorporating liquid crystal into silicon metasurface onto fluorescent glass substrate by Bohn et al.¹⁷⁹. By increasing the temperature above the critical temperature, liquid crystal experiments a transition from nematic state to isotropic state, accompanied by refractive index change. The background engineering results in the spectrum shift of Mie resonance supported by such a hybrid metasurface, causing the change of local photonic density of state that plays a dominant role in spontaneous emission enhancement. The magnetic (or electric) resonance nature of silicon metasurface also provides a nice playground to control the emission from trivalent lanthanide ions (i.e., Eu^{3+} and Er^{3+}) that has magnetic (electric) dipole transition in the visible or near-infrared wavelength range. By coating a Eu^{3+} doped polymer onto silicon metasurface, Vaskin et al. demonstrated that the magnetic (electric) emission enhancement factor from Eu^{3+} is 6.5(8) when the magnetic (electric) dipole resonance from metasurface is tuned to match the magnetic (electric) dipole transition at 590nm (610nm)¹⁸⁰. Note that large emission enhancement can be obtained by exciting the high-Q mode of quasi-bound-state-in-the-continuum via breaking the symmetry, as will be discussed in the application section of bound state in the continuum. Lasing becomes accessible when the resonant mode is integrated with the gain materials with a large quantum yield. By conformally growing the perovskite thin film onto the photonic crystal resonator¹⁸¹, Chen et al. successfully achieved coherent lasing 788.1nm with threshold as low as 68.5uJ/cm². Another example is the interlayer exciton lasing in atomically thin heterostructure $\text{WSe}_2/\text{MoSe}_2$, as demonstrated by Paik et al.¹⁸². Type II band alignment in heterobilayer $\text{WSe}_2/\text{MoSe}_2$ forms a three-level system and gives rise to long-lived interlayer excitons whose exciton and hole are located in the separate layers, facilitating the establishment of population inversion. Thus, such a heterostructure can serve as gain materials. By transferring heterobilayer onto Si_3N_4 metagrating that supports a high-Q mode, an atomically thin coherence laser is achieved with a threshold low to 0.18uW. Also, as a key feature of justifying laser, extended spatial coherence was experimentally confirmed.

Strong coupling

Benefiting from the considerable field enhancement of Mie resonance, the dielectric nanoresonator has also found promising applications in enhanced strong coupling between Mie mode and exciton of organic molecules and 2D transition metal dichalcogenide monolayer. 2D transition metal dichalcogenide has been regarded as an excellent platform to realize strong coupling at room temperature due to its large binding energy of exciton. The simplest example of Mie resonance induced strong coupling is to integrate a single silicon nanosphere with organic molecules and transition metal

dichalcogenide monolayer^{183–185}. Wang et al. perform both theoretical and experimental studies on the resonant coupling between the exciton of 1L WS₂ shell and magnetic dipole resonance in silicon nanosphere core¹⁸³. Although anticross behavior in the scattering spectrum was observed with mode splitting 43 meV, the absence of mode splitting in the absorption spectrum suggests the weak coupling instead of strong coupling in such a hybrid system. Additionally, the Fano interference between magnetic dipole resonance and exciton leads to unidirectional light scattering. In the same year, Lepeshov et al. theoretically predicted the strong coupling with Rabi splitting >110meV in 1L WS₂ wrapped around silicon nanosphere¹⁸⁴. The Rabi-splitting is further improved to 208meV by replacing the background medium with water. The measured Rabi splittings are 49.6 and 86.6meV when the hybrid structure is embedded into air and water, respectively. Tserkezis et al. conducted a comprehensive theoretical calculation on the strong coupling of silicon-core and organic molecules or transition metal dichalcogenide shell¹⁸⁵. The rich optical modes from such a core-shell structure enable a large a Rabi splitting 150-200meV, comparable to plexciton. The low-loss nature of silicon also allows for observing Rabi oscillation over several periods in a strongly coupled Mie-exciton system. Although a single dielectric nanosphere offers many conveniences of studying strong coupling due to analytical solutions, it might be more appealing to develop an all-dielectric metasurface to realize strong coupling from real application perspective. By transferring 1L-WS₂ and WSe₂ onto the Si₃N₄ metagrating, Zhang et al. demonstrated the strong coupling at room temperature between the exciton and leaky modes supported by the metastructure¹⁸⁶. Due to the high-Q factor of the leaky mode, both PL and reflection spectrum show anticrossing (Fig.14g-h), signifying the strong coupling between the emitter and cavity mode. The retrieved maximum Rabi splittings are 22.2meV for 1L-WS₂ and 17.6meV for 1L-WSe₂, respectively. Although they are smaller than the Rabi splitting in the hybrid plasmonic/1L transition metal dichalcogenide system, the values could be boosted to more than 70meV using a multilayer hBN/1L-WS₂ structure that is embedded into the center of Si₃N₄ grating¹⁸⁷. Later, exciton-polariton has also been reported in a hybrid system made of 2D Si₃N₄ metasurface and 1L-WSe₂¹⁸⁸. Analyzing the anticrossing in PL and reflection spectrum gives Rabi-splitting 18meV. Moreover, it has been demonstrated that both polariton dispersion and far-field emission patterns could be engineered by arranging the meta-atoms. Besides, Wang et al. explored the Mie surface lattice resonance in a silicon NP array to study the strong coupling between 1L-WS₂ and Mie modes¹⁸⁹. Both the theoretical and experimental results show that only electric Mie-resonance could be strongly coupled to the exciton in monolayer WS₂ with Rabi-splitting 32meV. Note that the strong coupling is not limited to two-dimensional materials. Two independent groups proposed to use an all-dielectric metasurface to realize the strong coupling of J-aggregated organic molecules^{190,191}. The high-Q factor of collective surface lattice resonance directly results in a large Rabi-splitting around 200meV for both TE and TM polarization. Because perovskite exhibits large exciton binding energy and high emission efficiency, Dang et al reported the experimental demonstration of strong coupling with perovskite-metasurface¹⁹² (Fig.14i-j). Clear anticrossing was observed between photonic mode and exciton for both PL and reflection spectrum, verifying the strong coupling with Rabi-splitting >200meV.

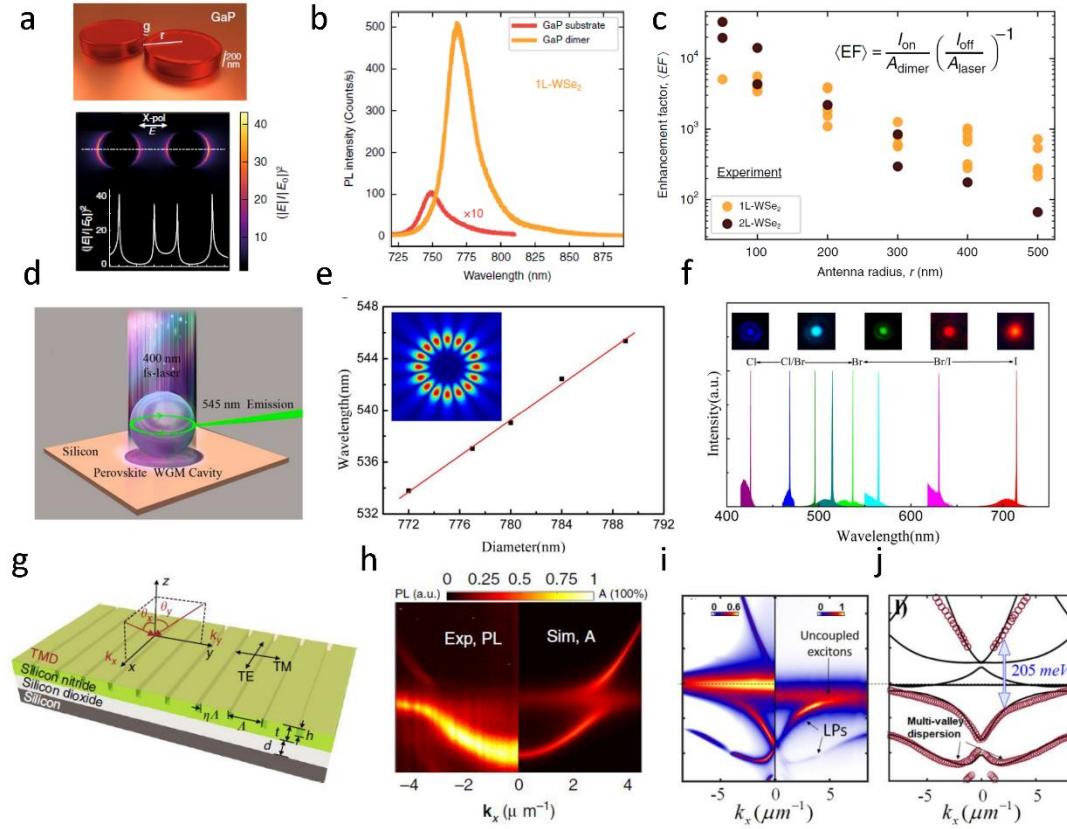


Fig.14. Enhanced light emission and strong coupling by leaky modes. (a) The top panel is a schematic drawing of GaP dimer nanoantenna. The bottom panel is electric field intensity distribution at resonance. (b) PL spectra of WSe₂ on top of GaP substrate and GaP dimer. (c) Measured PL enhancement factor in 1L-WSe₂ and 2L-WSe₂ as a function of the antenna radius. (d) Schematic of single-mode lasing from single CsPbBr₃ microsphere. (e) Lasing wavelength vs sphere diameter. (f) Tunable laser spectra by varying the composition of perovskite. (g) Schematics of transition metal chalcogenide monolayer strongly coupled to Si₃N₄ metagrating. (h) Measured and simulated PL spectra for a hybrid system. (i) Simulated absorption and measured PL as a function of k_x . (j) Calculated exciton-polariton dispersion. (a-c) from Ref ¹⁷⁰. (d-f) from Ref ¹⁷³. (g-h) from Ref ¹⁸⁶. (i-j) from Ref ¹⁹².

2.4.4 Enhanced Nonlinear Harmonic Generation

Leaky modes in dielectric nanostructures have been extensively investigated for enhancing nonlinear harmonic generations. In recent years, developments in the physics of dielectric meta-optics suggest a novel mechanism of light localization by forming leaky modes based on the multipolar Mie resonances^{193,194}. In the vicinity of these formed leaky modes, the electromagnetic field of light can be strongly confined inside the dielectric nanostructures, suggesting a promising route to enhance light-matter interactions. It is widely known that Mie-type resonances can be tuned and tailored effectively via control over the size and geometry of the nanostructures^{193,194}. Thus, to facilitate the nonlinear optical processes such as second-harmonic generation (SHG), sum/difference frequency generation, third-harmonic generation (THG), four-wave mixing, etc^{195,196}, one can tune the leaky modes resonant to the pump or harmonic wavelength by carefully adjusting the geometric parameters of the nanostructures^{197,198}. The advantage of employing leaky modes for nonlinear optical processes is

2-fold. First, it can dramatically enhance the nonlinear emission intensity due to the near-field enhancement. Second, the generated leaky modes at the harmonic wavelengths, i.e., the nonlinearly generated multipoles and their interferences, can shape the harmonic radiation patterns, and help to realize unique characteristics of nonlinear emissions.

One type of widely studied leaky mode in dielectric nanostructures is the magnetic dipole (MD) resonance characterized by circular displacement currents excited inside the nanostructures¹⁹⁹. MD resonance is associated with strong near-field enhancement and large mode volume thus is beneficial for boosting the nonlinear light-matter interactions. By adjusting the MD resonant position at the pump wavelength, researchers have demonstrated its ability and potential to enhance nonlinear generations^{200,201,210–219,202–209}. The field localization and enhancement near the MD resonance result in a strong enhancement of nonlinear harmonic generations. Take a silicon nanodisk as an example, pumping light at the MD resonance leads to two orders of magnitude enhancement of the third-harmonic intensity with respect to unstructured bulk silicon (Fig.15a-b)²⁰⁰. For second-order nonlinear processes, GaAs, AlGaAs, LiNbO₃, have been used to enhance the second harmonic generation using leaky modes supported in dielectric nanostructures^{202,203,212–217,204–211}. By exciting a strong MD resonance in the near-IR wavelength range, the SHG conversion efficiency has been theoretically predicted to be larger than 10^{-3} from a single AlGaAs nanodisk with a pump intensity of $I_0 = 1\text{GW}/\text{cm}^2$ (Fig.15c)²⁰², and later the nonlinear conversion efficiency exceeding 10^{-4} has been reported experimentally (Fig.15d)²⁰⁴. Enhanced SHG using GaAs metasurface supporting MD resonance has been experimentally demonstrated 100 times higher conversion efficiency than the conversion efficiency at the electric dipole resonance, four orders of magnitude higher than the SH signal obtained from unpatterned GaAs²⁰⁵. Besides, by exciting leaky modes of different multipolar nature at the harmonic wavelengths, radially-polarized or azimuthally-polarized vector beams and other complex beams can be generated^{204,207,213,216}.

The leaky modes supported by an individual single NP can be further improved by grouping several NPs together to form dielectric dimers, trimers, or other oligomers^{201,220,221}. The coupling between these closely-placed NPs substantially enhances electromagnetic fields via hybridization of individual Mie resonances. Meanwhile, it provides an additional degree of freedom to engineer the linear and nonlinear light scattering properties. By placing three silicon nanodisks arranged in the form of a trimer with varying distances between them, researchers have experimentally observed a pronounced reshaping of the third-harmonic spectra due to the interference of the nonlinearly generated waves augmented by an interplay between the electric and magnetic dipole resonances, as illustrated in Fig.15e²²⁰. Similarly, when placing two identical silicon NPs adjacent to each other, the hybridized leaky mode with a ‘hotspot’ in the gap between the two NPs can significantly enhance the nonlinear emission and the multipolar harmonic modes generated by the dimers further allow the shaping of the directionality of nonlinear radiations²²¹.

Among the various leaky modes supported by the dielectric nanostructures, some of them are not able to excite directly under linearly polarized beam illumination. This can be explained by the fact that the multipolar structures of these leaky modes do not share any multipole contents in common with the linearly polarized pump light. In such cases, vector beam excitation has been employed^{222–226}. It has been shown that by tailoring the vectorial structure of the pump light, not only the harmonics can be significantly enhanced, but also one can control both the strength and polarization composition of the excited harmonic fields. Similarly, nonlinear structured light with a special polarization feature can be

generated by addressing a different type of multipolar content selectively (Fig.15f-g)^{224,226}.

Another interesting feature of leaky modes is, the interference between different leaky modes can suppress the scattering and realize non-radiating configurations such as an anapole state. In dielectric meta-optics, the electric or magnetic anapole states originate from the overlap of a co-excited Cartesian electric dipole and toroidal dipole moments, Cartesian magnetic dipole, and mean radius distribution component of the magnetic dipole, respectively^{227–229}. This results in the cancellation of their scattering contributions in the far-field while exhibiting strong near-field enhancement inside the nanostructures, providing a novel platform for enhancing nonlinear interactions at the nanoscale dielectrics^{230–236}. The anapole state was first employed for nonlinear conversion in Ge nanodisks in 2016, as illustrated in Fig.15h²³⁰. At the spectral region of the anapole state, a pronounced valley in the scattering cross-section. Meanwhile, the electromagnetic field energy is concentrated inside the Ge nanodisk. The experimentally measured THG conversion efficiency reaches 0.0001%, reaching four orders of magnitude higher than the case of an unstructured Ge reference film. A further improvement of anapole state excitation can be obtained through geometry optimization, such as using a metal-dielectric nanostructure consisting of Si nanodisk as a core and a gold ring as a shell (Fig.15i)²³¹. Such a configuration utilise the gold ring to boost the electric field enhancement at the anapole state inside the Si nanodisk due to its plasmonic properties. The THG conversion efficiency via this configuration reaches 0.007% at a third harmonic wavelength of 440 nm. A similar configuration has been employed to AlGaAs nanodisk²³². By placing a gold ring around the AlGaAs nanodisk, the excited anapole state enables the improvement of both the second- and third-order nonlinear emissions from AlGaAs, with measured enhancement factors of about 30 and 15, respectively. Furthermore, by employing a metallic mirror under the dielectric NPs, a novel characteristic of the anapole state can be achieved through the spatial overlap of resonantly excited Cartesian electric and toroidal dipole modes (Fig. 15j)²³³. Such a configuration can produce a giant near-field enhancement to facilitate the nonlinear process, and meanwhile, the mirror surface boosts the nonlinear emission via the free-charge oscillations within the interface, equivalent to producing a mirror image of the nonlinear source and the pump beneath the interface. As a result, a THG conversion efficiency of 0.01% from a mirror-enhanced Si anapole resonator has been experimentally obtained.

Benefiting from the leaky modes in dielectric nanostructures, the field of nonlinear nanophotonics has witnessed rapid progress in recent years^{237,238}. The enhanced optical nonlinearities enabled by exciting the leaky modes have also been used for ultrafast modulation of light at the nanoscale^{96,97,239–241}, generation of quantum photon pairs^{212,242}, and infrared upconversion imaging²⁴³, etc.

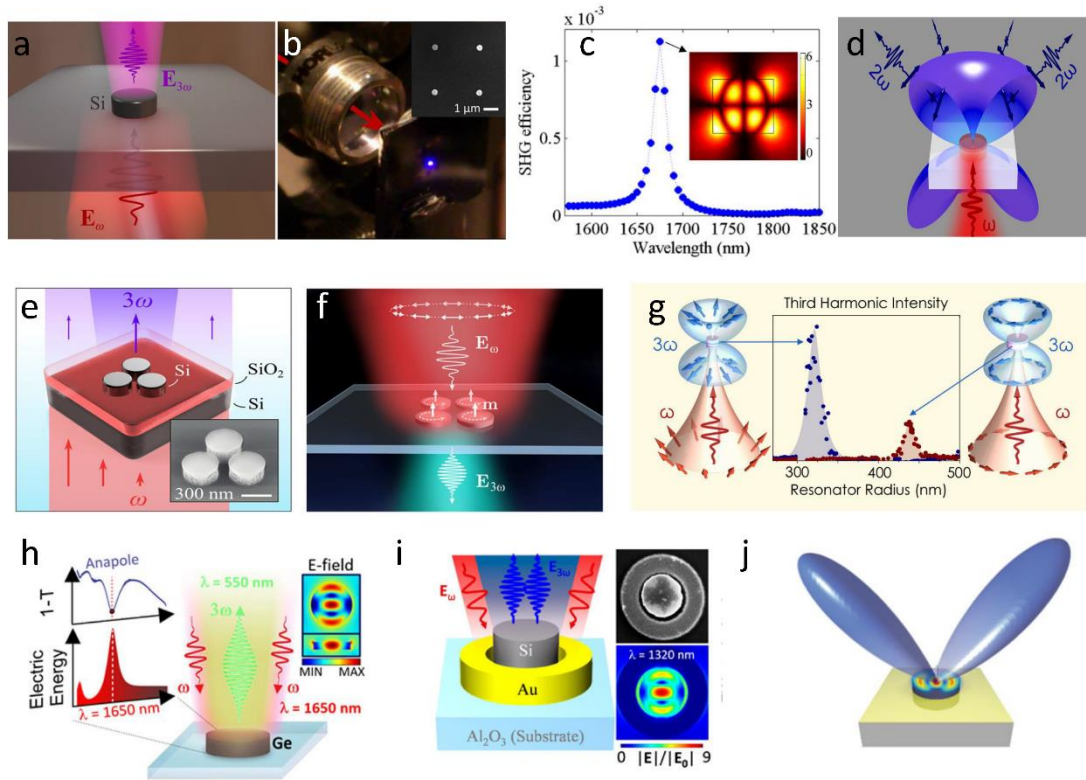


Fig.15. Enhanced nonlinear harmonic generation (a) schematic illustration of the THG process and enhancement from a Si nanodisk driven by MD resonance. (b) The photographic image of the eye-visible TH emission from the sample. (c) SHG efficiency as a function of pump wavelength from an AlGaAs nanodisk with radius 225 nm, height 400 nm. Inset: the normalized electric field at harmonics on a cross-section in the x-z plane at the center of the nanodisk. (d) Illustration of enhanced nonlinear vector beam generation from AlGaAs nanoantennas. (e) Illustration of the THG process in silicon nanodisk trimers. (f) Schematic representation of the nonlinear process from a Si oligomer excited with an azimuthally-polarised pump beam. (g) Selective third-harmonic generation in Si NPs with structured light pump. (h) Enhanced third-harmonic generation in a Ge nanodisk excited at the anapole state. (i) Schematic of the efficient THG from a metal-dielectric hybrid nanoantenna by exciting at the anapole state. Right upside: SEM image of the fabricated hybrid nanoantenna. Right downside: Calculated electric field distribution at the anapole state. (j) Calculated TH radiation from a Si anapole resonator placed on a gold substrate. (a-b) adopted from Ref ²⁰⁰. (c) from Ref ²⁰². (d) from Ref ²⁰⁴. (e) from Ref ²²⁰. (f) from Ref ²²⁴. (g) from Ref ²²⁶. (h) from Ref ²³⁰. (i) from Ref ²³¹. (j) from Ref ²³³.

2.4.5 Structural color

Color display constitutes an indispensable component in our daily life, from Television and mobile phone to laptop. Conceptually, the stimulation of photoreceptor cells in the retina results in the color perception of human eyes. The conventional way of rendering color is to utilise the pigments or dyes that absorb the photons at a given wavelength in the visible wavelength range. Although large-scale color generation can be achieved by the pigment or dyes, they suffer from either limited resolution or degradation with time in harsh conditions.

Recently, structural color enabled by nanophotonic structure has triggered extensive interest as it provides an alternative to achieving vivid and vibrant colors^{244–247}. Its origin can be traced to the bio-inspired structural color, such as the peacock's feature²⁴⁸ and Morpho butterfly's wing. A closer look at the microstructure of peacock feathers with SEM indicates that the different colored barblues are attributed to the 2D photonic crystals with partial photonic crystal bandgap, which can strongly reflect light. More examples of bioinspired structural colors can be found in a comprehensive review by Kinoshita et al.²⁴⁹.

The key to realising the structural color is to produce the required electromagnetic response (scattering, reflection and transmission) in a given wavelength range. The simplest way to engineer the reflection or transmission spectra is to explore destructive or constructive interferences from multilayer thin film. One of the typical examples is antireflection coating, for which the refractive index and the thickness must satisfy $n_2 = \sqrt{n_1 n_3}$ and $t = \frac{\lambda}{4n_2}$, respectively. However, when an ultrathin, highly lossy film (i.e. Ge) with a thickness of few nanometers (5–20nm) is coated on a thin metal film with finite optical conductivity, destructive or constructive interference still can be realized because of nontrivial phases from both highly lossy medium and the interface. Therefore, the reflection (or absorption) spectrum and color can be tuned even with several nanometers²⁵⁰, as demonstrated by Kats et al. The structural color arising from thin-film interferences can be thermally or electrically controlled when phase changed materials-germanium antimony tellurium alloy($\text{Ge}_2\text{Sb}_2\text{Te}_5$) are considered. Hosseini et al. found that multilayer thin film ITO/7nm GST/ITO on 100nm Pt/Si, quartz or flexible substrate can tune the color across the whole visible window²⁵¹. Such a multilayer structure can operate in both reflection and transmission modes.

Nevertheless, due to the highly lossy medium used in previous work, the reflection (or transmission) spectrum is quite broad and the color saturation may be low. To address this challenge, ElKabbash et al. proposed a Fano-resonant optical coating strategy for shrinking the linewidth of resonance²⁵². In their design, a broadband light absorber consisting of ultrathin highly lossy film on highly reflective metallic substrate, is weakly coupled to a narrowband light absorber made of metal-dielectric-metal layered structure. The resonant coupling between these two structures directly results in the formation of Fano-type reflection or absorption spectrum and different colors. Interestingly, the same color can be generated at transmission and reflection modes. Thin-film coating represents a cheap and versatile technology because it can be produced on a large scale. However, structural colors enabled by thin-film coating have a limited color gamut, low brightness and color saturation. Also, it might be very challenging to produce a complicated image with a high resolution because the thickness must be tuned to generate different colors.

Subwavelength nanostructure has emerged as a powerful platform for manipulating light at the nanoscale and tailoring the reflection or transmission spectra as it supports optical resonance (i.e., plasmonic resonance or Mie resonance). Many efforts have been devoted to structural color generation by exploiting plasmonic resonance. The major advantage of plasmonic resonance is that it can confine the electromagnetic field beyond the diffraction limits, significantly improving the resolution of structural color resolution. Also, its resonant wavelength can be tuned easily by the size of metallic NPs. Recent progress on structural color by plasmonic nanostructures has been reviewed by different groups^{245–247}.

Despite so many advantages plasmonic color generation enjoys, the large intrinsic loss from metals inevitably broadens the plasmonic resonance, limiting the color saturation. On the other hand, the prohibitive price of noble metals (i.e., Au and Ag.), may hinder the larger scale applications. High-index semiconductors, such as Si and GaAs, are an ideal platform for realising CMOS-compatible structural color because they also support electric and magnetic Mie-type resonances (also called leaky modes). On the other hand, the intrinsic material loss is very low compared to the counterpart of metallic nanostructures. These combined properties enable scientists to develop the optical resonance at an arbitrary wavelength with a high-Q factor, which is the key ingredient of achieving structural color with high saturation and large color gamut^{253,254}. Also, the high-index, such as Si~4, enables the electric field of optical resonance to be tightly confined inside the nanostructures. This is beneficial to maintain the structural color's resolution. The initial effort of Mie-resonance-enabled structural color can be dated back to 2010, where Cao et al. demonstrated experimentally that different colors could be generated in a single silicon NW due to resonant scattering⁷⁴. In 2012, Kuznetsov et al. revealed that a single silicon NP could produce a robust color by simply varying the radius of nanosphere¹⁹⁹. The fundamental physics behind it is that magnetic Mie resonance has been continuously tuned from 470nm to 720nm as the diameter varied from 100nm to 270nm. Although a single silicon nanostructure can generate different colors, it still has limitations. Firstly, the scattering intensity is so weak that can only be observed in dark-field scattering microscopy. Secondly, with the increasing size of the NP, except for MD resonance, other multipolar Mie resonance including ED and EQ resonance, are also excited. The interference among them makes it difficult to produce the pure red color. Thirdly, the intrinsic loss becomes considerable and could not be neglected at short wavelengths below 450nm. This also makes the blue color generation becomes less efficient. Therefore, much attention has been turned to an array of dielectric metasurfaces for structural color generation. Proust et al. demonstrated color printing with all-dielectric silicon metasurface²⁵⁵. In this work, low-order electric and magnetic Mie resonances supported by silicon NPs are carefully engineered to manipulate the light scattering in the visible wavelength range, giving rise to a large palette of colors. Flauraud et al. performed a systematic study on the comparison of structural color generated by metallic (i.e., aluminium and silver) and dielectric (silicon) nanoresonators²⁵⁶. They found that the Al NPs can cover the largest wavelength range but has low-Q factor while Ag NPs show improved Q-factor but limited tunability.

In contrast, Mie resonance supported by Si NPs can simultaneously cover the whole visible wavelength range and have high-Q factor. By harnessing electric and magnetic resonance, they successfully demonstrated large-scale painting reproduction based on silicon nanodisk array. After acquiring the knowledge of Mie resonator on color generation, different types of Si Mie resonator design have been theoretically proposed and experimentally realized to produce high-quality structural color²⁵⁷⁻²⁶⁰. For example, Nagasaki et al. realized polarization-dependent color generation with dual-color pixel in a silicon nanoblock array²⁵⁹. Even a single element can generate individual colors, and the spatial resolution is pushed up to 85,000dpi.

Although a wide range of colors has been successfully imprinted by Si Mie resonators, their performance is still far away from satisfactory because of the limited color saturation, brightness, gamut and resolution. A more advanced design has been proposed to address these issues. For example, Dong et al. demonstrated an improved color gamut (121% of sRGB) but retained the print resolution (100,000 dpi) by introducing an index-matching layer Si₃N₄ between silicon nanodisk array and silicon substrate²⁶¹. The sandwich layer Si₃N₄ acts as an antireflection coating layer to eliminate the unwanted

reflection from substrate, thus sharpening the reflection peak. This effect is also explained by Kerker's condition, where magnetic dipole and electric dipole have equal amplitude and phase from multipole decomposition. Instead of patterned amorphous silicon on Si_3N_4 /silicon substrate, Yang et al. developed an alternative strategy of realising high-performance structural color with simultaneously large gamut, high saturation, high brightness and high resolution by utilising a single layer of Si metasurface²⁶². As shown in Fig.16a, the single crystalline silicon on sapphire is patterned as Mie resonators array to create a tunable resonance across the visible wavelength range. Similar to previous work, a refractive index matching layer, such as dimethyl sulfoxide (DMSO) and PMMA, is introduced on top of the metasurface to suppress the background reflection from the substrate and sharpen the resonant peak. Fig.16b-c shows the reflection spectra of Si metasurface in the air and DMSO. When embedding metasurface into DMSO, the Mie resonance shows redshift and simultaneously the full-width-half-maximum reduces compared to the case of air. Besides, the background scattering is suppressed to almost zero due to the antireflection coating layer. The corresponding structural colors are plotted in CIE color maps and shown in Fig.16d. The color gamut area is up to 181.8% of sRGB, 135.6% of adobe RGB and 97.2% of Rec.2020 for metastructure in DMSO. Furthermore, due to the large refractive index contrast between silicon and background, the structural color is still distinguished even when pixel size reduces to 2×2 Si nanodisk array. Thus, the print resolution approaches diffraction limit. The superior performance of structural color enabled by such a metasurface is manifested by the more vivid peacock image in DMSO than in air, as shown in Fig.16e-f. Other index matching layer, such as liquid crystal or PMMA, can play similar role as DMSO in obtaining vivid and vibrant colors with large color gamut, high saturation, high brightness and high resolution. The all-silicon-based structural color is compatible with current CMOS technology and paves the way toward practical commercialisation

Although the intrinsic material loss for Si is much lower than plasmonic nanostructure, it still poses some limitations on the amplitude of resonance peak and color saturation. Therefore, other lossless materials with relatively high refractive index, such as Si_3N_4 ($n \sim 2.0$)²⁶³⁻²⁶⁵ and TiO_2 ($n \sim 2.2$)²⁶⁶⁻²⁶⁸, have been widely used to develop structural color. By applying Rayleigh anomalies that suppress high-order Mie resonant mode at short wavelengths, Yang et al. successfully demonstrated the highly saturated structural color with a wide gamut and high resolution ($>10,000\text{dpi}$) based on Si_3N_4 metasurface²⁶⁵. Fig.16g shows the reflection spectra of dielectric metasurface on quartz with varied refractive index. It can be found that magnetic dipole lattice resonance always maintains a large value approaching unity regardless of the refractive index of nanoresonator because this resonance is zero-diffraction dominated. However, the shoulder peaks at shorter wavelength are quenched due to strong Mie-resonator-substrate coupling when the refractive index is reduced from 2.5 to 2.0. The successful suppression of high-order Mie resonance at shorter wavelength guarantees the single sharp peak in the whole visible wavelength range and the high purity color. Following this designing strategy, three typical colors have been successfully constructed both theoretically and experimentally with reflection spectra shown in Fig.16h. The excellent performance of structural color is evidenced by a larger gamut compared to sRGB, as shown in Fig.16i. Furthermore, a rainbow-like character "NANO" shown in Fig.16j, was fabricated with such a Si_3N_4 metasurface by varying the nanocube resonator size and lattice constant. The smallest pixel size is $2.5\mu\text{m} \times 2.5\mu\text{m}$, representing the resolution of 10160 dpi. In addition, it is worth pointing out that structural color does not only work for reflection and transmission mode but also operate at lateral incidence via long-range dipole interaction (Fig.16k). Consequently, such a metasurface may find applications in eyewear display for augmented reality. TiO_2 is another transparent materials with

high-index in the visible range. Sun et al. demonstrated the first structural color based on TiO_2 metasurface by engineering the electric and magnetic resonance²⁶⁶. The bright and saturated color from such metastructures stems from the single reflection peak with high intensity (up to 64%) and reasonably narrow linewidth (30nm). Additionally, the structural color can still be clearly distinguished when the metasurface reduced to 4×4 arrays, signifying that the resolution can be up to 16000 dpi. To further improve the color saturation based on TiO_2 and Si_3N_4 , Yang et al. developed an advanced design that consists of patterned $\text{SiO}_2/\text{TiO}_2/\text{Si}_3\text{N}_4$ metasurface on silica substrate²⁶⁷. Both SiO_2 and Si_3N_4 layers function as antireflection coating layers, which help to suppress the high-order Mie resonance at short wavelength and eliminate the background reflection. The measured reflection efficiency are ranged between 62.3% and 88.1% when period varies from 300 to 400nm. The retrieved color gamut are found to be 171% of sRGB, 127% of adobe RGB, 90% of Rec.2020. The highly saturated color is even maintained in 4×4 arrays ($1.4\mu\text{m} \times 1.4\mu\text{m}$ pixels), representing the resolution >18000 dpi.

Note that the above works are passive generation of structural colors. Once this structure is fabricated, its function can no longer be changed. In real applications, it is desirable to show dynamical control on the structural color. Frank et al. summarize the recent advances of dynamical plasmonic color generations²⁴⁵. Here, we focus on discussing active control of structural color based on all-dielectric metasurfaces²⁵³. Usually, structural color can be dynamically tuned by mechanical strain^{99,100,269}, electric gating⁷⁸, chemical reaction²⁷⁰, thermal heating and laser shining²⁷¹. Through transferring high-contrast silicon metastructure on a transparent, flexible polydimethylsiloxane (PDMS) membrane, Zhu et al. realize a tunable structural color from green to orange²⁶⁹. Unlike most works discussed above, structural color enabled by such metastructures can be observed at large angles because -1^{st} order diffraction dominates the reflection. In 2019, Zhang et al. demonstrated a mechanically tunable structural color by transferring TiO_2 -metasurface onto a flexible substrate-polydimethylsiloxane (PDMS)¹⁰⁰. When the strain increases from 0 to 40%, the optical resonance can be dynamically tuned from 450nm to 650nm, almost covering the full spectrum of visible wavelength ranges. In fact, tunable Mie resonance was reported with TiO_2 metasurface on PDMS substrate in 2015 by Gutruf et al. although they did not record the structural color⁹⁹. Therefore, structural color can be effectively tuned from blue to red via strain engineering. Although color gamut is not as large as the previously reported one, the larger tunability enables it to find applications in encryption. Further improvement on the structural color performance may require topology optimization. If such a TiO_2 metasurface is embedded into an environment with different refractive index, an obvious resonance shift should be expected as the eigenfield is mainly localized in the gap between unit cells. Following this strategy, Sun et al. reported a tunable structural color in the real-time domain by integrating TiO_2 metasurface onto microfluid channels²⁷². The response time is as fast as 16ms. Structural color can also be switched on/off by TiO_2 metasurface²⁷⁰, as demonstrated by Wu et al. The fundamental physics behind it is to tune the refractive index of TiO_2 via ion implementation by ICP, especially the imaginary part of the refractive index. TiO_2 metasurface can be converted into black TiO_2 via H^+ implementation and recovered by O^- implementation. Thus, applying ion implementation on TiO_2 metasurface may serve as a viable way of writing and erasing colors. Laser pulse is another way of tuning the structural color. Zhu et al. demonstrate massive production of structural color by resonant laser printing based on Ge-metasurface²⁷¹. Due to resonance enhanced band-to-band absorption in Ge, the local temperature of Ge metasurface is elevated to 1200K by pulse laser irradiation. This directly results in the morphology changes and color tuning. Modern display

technologies request the dynamical manipulation of structural color by electrical gating. In 2019, Holsten realized a electrically reconfigurable Si metasurfaces with fast speed ($>10^5$ Hz), where temporal color mixing has been created in a micro-electrical mechanical system⁷⁸. Note that all above devices only have a single functionality. Through judiciously engineering the destructive interference and leaky mode resonances in different environment, Yang et al. successfully demonstrated a dynamic bifunctional metasurface that enables simultaneous metahologram and structural colors. By illuminating the red and blue laser at the same time, different hologram images are shown if the solvent DMSO flow through the metasurface. This interesting functions could find immediate applications in encryption. Although such devices show fantastic performance on switching image from one to the other, they can only operate at two pre-designed wavelength. The operating wavelength may be extended by incorporating the design on achromatic metalens into structural color design. Also, the efficiency could be improved by adopting an advanced design.

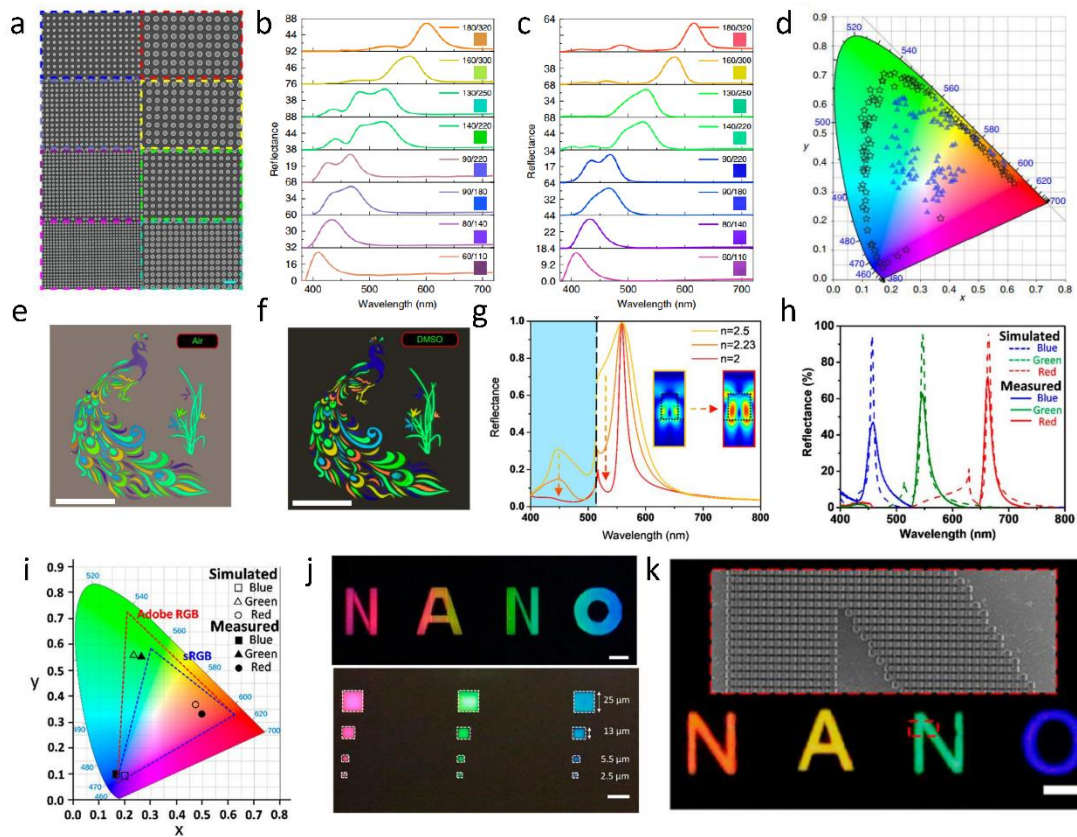


Fig.16. Structural color enabled by leaky mode resonance. (a) SEM image of silicon metasurfaces. (b-c) Measured reflection spectrum of metasurfaces embedded in the air and DMSO. (d) Measured color palette for silicon metasurfaces in air and DMSO. (e-f) Optical image of the metasurfaces in air and DMSO. (g) Simulated reflection spectra of dielectric metasurfaces with varied refractive index. (h) Simulated and measured reflection spectra for Red, Green and Blue color. (i) Color gamut of Si₃N₄ metasurface. sRGB and Adobe RGB are plotted as references to make a comparison. (j) Optical image of character NANO and colorful square created by Si₃N₄ with different size. (k) Optical image of character NANO under lateral illumination. (a-f) from Ref ²⁶², (g-k) from Ref ²⁶⁵.

3. Bound states in the continuum

As a particular type of leaky modes, BIC has received tremendous attentions in the past decades and triggered extensive interests across the photonic and acoustic community because it has an infinite Q-factor and a zero radiative decay rate despite of embedding into the radiation continuum. The direct consequence of ultrahigh Q-factor in QBICs is the extreme field confinement, promising many exciting applications on enhanced light-matter interactions. In this section, we review the most advances of BICs and QBICs from fundamental principles to applications.

3.1 BIC in a single structure

3.1.1 QBIC in a single dielectric structure

As a typical non-hermitian open system, high-index dielectric structures support a number of leaky modes (or QNMs) with either electric or magnetic characteristics. In section 2.3.1, we have discussed the general mode properties in a single dielectric nonspherical nanostructure. The real part of eigenvalue for a given mode shows a linear dependence on the size ratio. Also, in section 2.3.4, it is derived that BIC or QBIC could be constructed by proper engineering the complex coupling. The signature of BIC or QBIC's emergence is the crossing or avoided crossing of resonant frequencies. Here, we illustrate that high-Q mode, also noted QBIC, could be found in such an isolated dielectric NP thanks to the simple linear relationship between eigenvalues and size ratio.

In 2006, Wiersig reported the high-order QBICs in an open optical microcavity with different shapes (i.e. rectangle, ellipse and semistadium)²⁷³. Such QBICs have a diamond-shaped eigeifield profile. Their formation is ascribed to the diffraction at microcavity corner leading to the complex coupling. QBICs (or high-Q supercavity modes) also have been demonstrated in a single dielectric cylindrical resonator⁴⁹ by Rybin et al. They are interpreted by the strong coupling between Mie-like modes and Fabry-Perot-like modes that leads to Friedrich-Wintgen-like interferences²⁷⁴, as demonstrated by Bogdanov et al. Moreover, they also establish a direct link between the high-Q resonances and the peculiar feature of Fano resonance in the scattering cross-section spectrum. Multipole decomposition indicates that far-field radiation experiences drastic change due to the multipolar conversion from low order to high order²⁷⁵. The subtle connection between Q-factor and radiation pattern is in favour of realising unidirectional radiation with such high-Q modes, which belongs to the generalised Kerker condition among different multipole channels. Huang et al. unveiled a universal rule of finding out all QBICs in a single non-spherical dielectric nanocavity²⁷⁶ (i.e. rectangular wire, cylindrical disk with finite thickness and cuboid). Instead of labelling the high-Q and low-Q modes as Mie-like modes and Fabry-Perot-like modes, the leaky modes supported by a single rectangular NW, for example, are noted as $TE_{m,l}$ (m and l are the number of field maximum along x and y axis) when the electric field is perpendicular to the cross-section of structure in xoy plane. Thanks to the linear relationship between the real part of eigenvalues and size ratio, all QBIC modes can be easily found through constructing the avoided crossing (or crossing) between a pair modes, such as $TE_{m,l}$ and $TE_{m+2,l-2}$ or $TE_{m,l}$ and $TE_{m-2,l+2}$. Fig.17a-b shows a represented example of a pair high-Q mode TE_{34} and low-Q modes TE_{52} in a single rectangular NW with $n=4$. Indeed, the real parts of eigenvalules of two modes display avoided crossing at $R=0.855$, around which the Q-factor of mode TE_{34} reaches maximum 1309 while the Q-factor of mode TE_{52} decreases to minimum 33. Fig.17c shows the electric field evolution of two modes around the critical size ratio. An interesting feature is that QBIC has a similar field profile of mode TE_{51} in a

single circular NW. Such a coincidence suggests that mode TE_{m1} may be viewed as a special type of QBIC. This is true when we consider a single elliptical NW with a size ratio defined as $R=b/a$, where a and b are the semi-long and semi-short axis of the ellipsis. QBICs TE_{m1} or TM_{m1} always happen at circular NW with $R=1$, around which avoided crossing could be found. As a typical example, Fig.17d-f shows the formation of high-Q mode TE_{31} and low-Q mode TE_{12} by sweeping the size ratio. This rule is so general that it could be applied to 2D rectangles or ellipsis with TM polarization and 3D cases, such as ellipsoids, cylinder nanodisks and cuboids. The emergence of QBICs at a particular size ratio is explained by the suppressed far-field radiation in the corresponding multipole eigenchannels. Meanwhile, QBIC only occurs when the electric (or magnetic field) is quenched to a minimum in momentum space. Here, we must stress that an ideal BIC does not exist in a single dielectric structure with a finite refractive index because there is always an outgoing radiative wave in the far-field. Thus, all work in a single NP focus on QBIC. The experimental demonstration of QBIC in a single dielectric structure has been done in the microwave and near-infrared wavelength range. By taking advantage of the high-permittivity of lanthanum aluminate–calcium titanate ($LaAlO_3$ – $CaTiO_3$) in microwave range, Odit et al. reported an ultrahigh Q-factor up to 1.25×10^4 in a subwavelength cylindrical resonator²⁷⁷. The Q-factor in near-infrared has also been demonstrated in a subwavelength silicon NW and cylindrical AlGaAs resonator with values 200~400^{276,278}.

Note that the strategy of finding QBIC by constructing avoided crossing does not only work in a single structure but also works for multi meta-atoms. Pichugin et al. demonstrated that the Q-factor of QBIC could be enhanced by one-order of magnitude with two coaxial dielectric disks²⁷⁹. Later, they found that the Q-factor of QBIC mode shows three orders of magnitude improvement compared to the case of a single isolated disk by simultaneously engineering the distance between twin disks and aspect ratio²⁸⁰. Also, an interesting finding is that such QBICs have similar eigenfield profiles to the spherical Mie resonant mode with a high refractive index. Further increasing the number of coaxial nanodisks leads to an ultrahigh-Q up to 10^5 for three disks and 10^6 for four disks²⁸¹. The same phenomenon also happens in the case of three NWs, where the Q-factor of one mode reaches a local maximum of 160 at a certain distance. The Q-factor is further increased to 1800 when both nanostrip ends are coated with silver²⁸². Taghizadeh et al. push the limit of Q-factor to 53,100 at 1550nm with three NWs²⁸³.

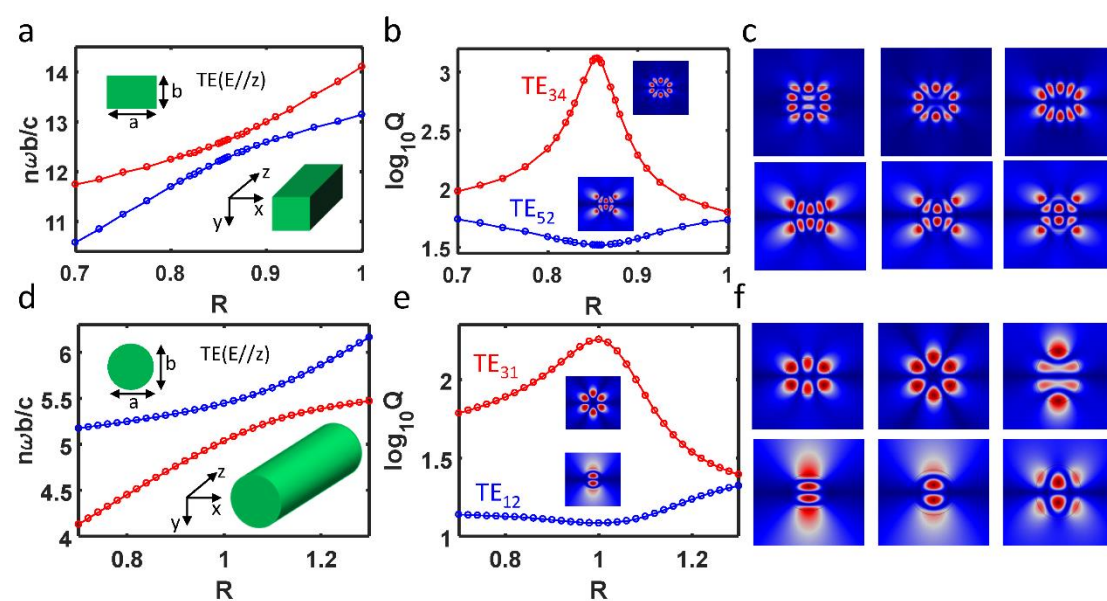


Fig.17. (a) Normalized eigenfrequency of leaky modes TE₃₄ and TE₅₂ vs size ratio $R=b/a$. (b) Q-factor vs size ratio R . (c) Eigenfield evolution of leaky modes TE₃₄ and TE₅₂. (d) Normalized eigenfrequency of leaky modes TE₃₁ and TE₁₂ vs size ratio $R=b/a$ in a single elliptical NW with $n=4$. (e) Q factor as a function of size ratio $R=b/a$. (f) Eigenfield evolutions of leaky modes TE₃₁ and TE₁₂. (a-c) from Ref ²⁷⁶.

3.1.2 BIC in single dielectric-metallic structure

An open cavity could support BICs (also noted as embedded states) if a dielectric structure is integrated with zero-index metamaterials. In 2014, Silverinha presented the first study of light trapping in an open cavity²⁸⁴ consisting of a dielectric sphere core layer and epsilon-near-zero (ENZ) shell layer. ENZ is realized by a metal at plasma frequency $\omega=\omega_p$, whose permittivity is described by $\epsilon=1-\omega_p^2/(\omega(\omega+i\omega_c))$. Ideal BIC occurs only at $\omega=\omega_p$ for lossless plasmonic structure. Meanwhile, the frequency $\omega=\omega_p$ must match the resonant frequency of the dielectric sphere surrounded by the perfect magnetic conductor. The transition from BIC to BIC could be induced by either introducing the nonzero collision frequency ω_c or tuning the inner radius of the dielectric sphere. Embedded states in a 3D subwavelength open cavity were also revealed by Monticone et al. in the same year²⁸⁵. In this work, the authors consider the layered nanosphere, which is comprised of a dielectric core layer ($\epsilon=1.5$) and two concentrated plasmonic shell layers with the same thickness but different plasma frequencies. Fig.18a shows the scattering cross-section spectrum mapping as functions of wavelength and aspect ratio $\eta_2=a/a_c$. Four BICs could be easily identified by checking the vanished linewidth. BICs 1 and 2 require the ultrathin shell ($\eta_2 \rightarrow 1$) and permittivity $\epsilon_3 \rightarrow 0$ (or $\epsilon_2 \rightarrow 0$) while BIC 3 requires $\eta_2 \rightarrow 0$ and $\epsilon_2 = -\epsilon_1/2$. Three BICs are challenging to realize in principle because it requires extreme structure parameters (i.e. vanished shell thickness or core diameter). For BIC 4, resonance with divergence lifetime happens for $\eta_2 \approx 0.597$ and $\epsilon_3 \rightarrow 0$. Fig.18b-c shows the electric field distribution at two different wavelengths $\lambda=0.995\lambda_c$ and $\lambda=\lambda_c$ for $\eta_2 \approx 0.595$. Only when the incident wavelength matches the critical wavelength can quasi-BIC be excited, evidenced by the strong field localisation inside the NP. A slight deviation from the critical wavelength makes quasi-BIC inaccessible.

In 2018, Monticone et al. generalised the concept of embedded state with the radiation continuum to the case of the 2D cylinder and 1D slab²⁸⁶. Like the 3D case, the dielectric cylinder is wrapped by the lossless plasmonic shell that enabled ENZ at $\omega=\omega_p$. To guarantee BIC in such a hybrid system, the dielectric cylinder should support a TE resonance with resonant frequency $\omega_0=\omega_p$. For a 1D dielectric slab sandwiched by the ENZ layers, BIC appears only when the Fabry-Perot resonance supported by the dielectric slab has the same frequency as the plasma frequency. Later, Sakotic et al. performed a thorough study on ENZ-dielectric-ENZ structure²⁸⁷. It is revealed that such a three-layer system could support both trivial and accidental BICs based on Berreman modes at normal incidence and oblique incidence, in analogy to symmetry-protected BIC and accidental BIC in photonic crystal slab. In fact, even a single slab made from zero-refractive index materials supports BIC²⁸⁸, such as ENZ, mu-near zero and impedance-matched zero indices, as reported by Li et al. Zhou et al. found that the strict requirement of geometry symmetry of realizing BICs could be lifted if multiple dielectric structures are placed into the zero-index medium²⁸⁹(Fig.18d-e). Thanks to the static-like field distribution, the total effective magnetic flux is nontrivial zero regardless of these structures' position, shapes and material parameters.

Here, it is necessary to comment that although ENZ could be realized by transparent conductive oxide, the intrinsic loss is inevitable to degrade the Q-factor of BIC. Also, the multilayer spherical or cylindrical structure is not easy to fabricate experimentally. Thus, currently most of BICs based on

zero-refractive index are theoretical works. More experiments should be done to prove the hypothesis. Note that the above discussion is limited to the single structure based on a hybrid ENZ-dielectric system. Some studies also show that an array of high-index NPs or photonic crystal slabs could support zero-index BIC, which is discussed next. Another slab system that supports BIC has been unveiled by Gomis-Bresco et al., where they consider a layer of anisotropic medium sitting on the isotropic or anisotropic substrate²⁹⁰. Through carefully engineering the ordinary and extraordinary refractive index of the core layer and substrate, and the thickness of the waveguide layer, the authors demonstrated the existence of BIC with pure TE polarization, TM polarization and full-vector polarization.

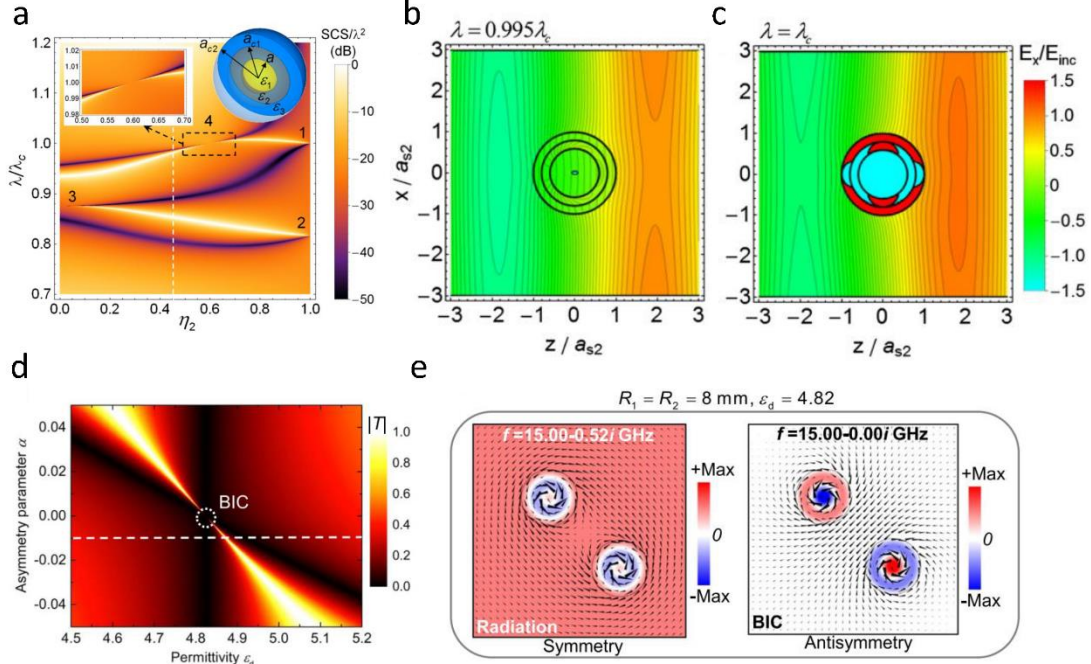


Fig.18. BIC in a single hybrid structure. (a) Normalized scattering cross-section mapping as a function of wavelength and the aspect ratio. (b) Electric field distribution at the wavelength $\lambda=0.995\lambda_c$ and $\lambda=\lambda_c$. (d) Transmission mapping as a function of permittivity and asymmetric parameters when two dielectric cylinders are embedded inside the zero-index-medium. (e) Eigenfield distribution of bonding and antibonding modes for two identical cylinders in zero-index-medium. (a-c) from Ref ²⁸⁵. (d-e) from Ref ²⁸⁹.

3.2 BIC in an array structure and its physical origin

3.2.1 BIC in an array of dielectric structures

An ideal BIC could be supported by all-dielectric photonic metastructures with periodic boundary condition along at least one direction. Their leaky mode nature requires the system should be open along one direction. Thus, most structures supporting BICs are 1D metagrating, 2D metasurfaces or photonic crystal slabs. According to the formation mechanism, BICs reported so far could be divided into four categories: symmetry-protected BICs, accidental BICs, Friedrich-Wintgen BICs and Fabry-Perot BICs. This section focuses on reviewing the most recent progress on these four types of BICs based on all-dielectric metamaterials.

Symmetry-protected BICs and accidental BICs

Perhaps symmetry-protected BIC is one of the most intensively studied BICs in the past decades because it can be easily accessed in many simple systems. As long as the array structure exhibits rotational symmetry, some leaky modes could decouple from the far-field, and thus are forbidden by external excitation. As an example, let us consider an array of period cylinders with electric field polarization along z direction²⁴. The schematic drawing is shown in Fig.19a. Due to the 180-degree rotational symmetry C_{2v} , such a simple grating structure supports many symmetry-protected BICs at Γ point, showing anti-symmetric field distribution along the periodic direction. The bottom panels of Fig.19a show two typical examples of BICs, BIC1-TE₁₁ and BIC2-TE₂₁. More typical structures that support symmetry-protected BIC are 1D rectangular grating, an array of dielectric spheres, a 2D dielectric metasurface and a photonic crystal slab with either square lattice or hexagonal lattice. As an ideal BIC is completely decoupled from the external environment, it could only be excited by breaking the symmetry in momentum space or geometry space, converting BIC into QBIC. For example, Lee et al. reported the experimental observation of QBIC Si₃N₄ photonic crystal slab by introducing the oblique incidence²⁹¹. It has been found that the reflection spectrum displays a Fano-profile at slightly off-normal incidence. The retrieved Q-factor of Fano resonance is as high as 10^4 . This is understandable because the field distribution along period direction no longer shows perfect anti-symmetry, causing the effective coupling between plane-wave excitation and QBIC mode. Another way to excite QBIC is to break the structure's in-plane symmetry. This methodology has been widely adopted to realize the high-Q mode at normal incidence. Different types of all-dielectric metasurfaces with meta-atoms like nanodisk with air hole^{292–294}, L-shape nanoresonator^{295,296}, nano-bar pair with different length^{297,298}, elliptical dimer^{299–302}, half elliptical and half circle disk^{303,304}, have been theoretically proposed and experimentally demonstrated. The measured Q-factor is ranged from several hundred to thousands. Later, Koshelev et al. presented a systematic study on such a structure asymmetry-induced QBIC in an all-dielectric metasurface³⁰⁵. By breaking the in-plane symmetry of the meta-atom, BIC is transformed into QBICs, whose Q-factor is inversely proportional to α^{-2} (Fig.19b), where α is the asymmetry parameter. Besides, Overvig et al. reported a comprehensive study on the selection rule of symmetry-protected BICs in different 2D-photonic crystal slab lattice types by breaking the in-plane symmetry³⁰⁶. From group theory perspective, six types of high symmetry BIC modes are explored in photonic crystal slabs with square lattice or hexagonal lattice. All of them could be selectively excited by introducing in-plane asymmetry. It is worth noting that QBIC does not only be excited by in-plane symmetry-broken but also out-of-plane symmetry-broken³⁰⁷. For practical applications, it is highly desired to realize active tuning on BICs. Fan et al. reported the dynamic control on the symmetry-protected BIC in the THz range through optical doping³⁰⁸. Eigenmode analysis indicates that the Q-factor could be modulated by two orders of magnitude. Almost at the same time, another work independently realized the active control on the QBIC mode by applying an optical pump and terahertz probe technique³⁰⁹. Experimental results show that such a reconfigurable metasurface allows for optical switching on a nanosecond scale. Malek et al. reported the thermal tuning of QBIC with a nonlocal silicon metasurface by exploring its high-Q nature³¹⁰. Kwon et al. experimentally demonstrated the active tuning of QBIC in a nano-electromechanical way³¹¹.

Another type of BICs that has been found in periodic structures is accidental BIC. Unlike symmetry-protected BIC occurring at Γ point, accidental BIC exists in the first Brillouin zone even when the symmetry broken has been induced by in-plane wavenumber. In 2008, Marinica et al. presented a theoretical prediction of accidental BICs in double-layer grating structures³¹², where the

BIC only happens at certain k_x . In 2013, Hsu et al. presented the theoretical prediction and experimental demonstration of accidental BICs in a dielectric photonic crystal slab with a square array of cylindrical air holes³¹³ (Fig.19c-e). Except for BICs at Γ point, another four BICs are found in the Brillouin zone. More specifically, they are distributed along k_x and k_y axis in momentum space and are fundamentally equivalent due to the square lattice symmetry belonging to C_{4v} group. The appearance of such BICs is attributed to the destructive interferences among several leaky channels. Their existence has been experimentally confirmed by fabricating a photonic crystal slab and measuring the angle-resolved reflection spectrum. Yang et al. presented an analytical coupled wave theory to explain the formation mechanism of accidental BICs³¹⁴. Indeed, the weighted destructive interference was enabled in the vicinity of accidental symmetry through the continuum coupling. Later, more studies revealed that this type of BICs also exist in 1D dielectric grating^{315,316}, 2D photonic crystal slab with hexagonal lattice^{315,317}, and 2D all-dielectric metasurface. However, we should emphasize that limited applications have been reported because this BIC usually happens at oblique incidence. More attention should be paid to exploring its full potential in practical applications. Note that accidental BIC is not a unique property of the photonic system. Also, it has been demonstrated in an open Sinai billiard by varying the shape of the cavity³¹⁸.

Friedrich-Wintgen BICs and Fabry-Perot BICs

BICs could be constructed by managing the destructive interference of two leaky modes. They can be classified as Fabry-Perot BICs and Friedrich-Wintgen BICs. The operation principle of Fabry-Perot BICs is explained as follows. It is well known that around the resonant frequency unity reflection could be made for a resonant structure that supports a well-separated leaky mode if the intrinsic loss is ignored. When two identical resonant structures are brought close to each other, BICs could be constructed by carefully arranging the distance between two resonators because these two resonators could serve as perfect mirror pairs. More specifically, a trapped wave is formed because of destructive interference when the accumulated propagation phase between resonators is the integer number of π . Fabry-Perot BICs have been theoretically demonstrated in bilayer stacked photonic crystal slabs³¹⁹ or grating structures^{312,320} (Fig.19h-i). The experimental verification has been done in coupled waveguide array³²¹ and two distant photonic crystal cavities³²². One may also build such a Fabry-Perot BIC by placing a resonator in front of a perfect mirror by taking advantage of mirror effects^{323,324}. For example, Hsu et al. successfully demonstrated that the surface leaky modes could be converted into a Bloch surface embedded state in the continuum by putting surface rods in front of a semi-infinite photonic crystal band structure that serves as perfect mirror³²³, where the operation frequency of surface resonance is localized in the bandgap of photonic structure. Destructive interference could be induced between two leaky channels: one is directly leakage into air and the other is the leakage from bouncing-back-wave from photonic crystal bandgap structure. Yu et al. harnessed the Fano interference between a half photonic crystal waveguide and photonic crystal cavity to realize a Fabry-Perot BICs³²⁴. Destructive interference is enabled by tuning the distance between the photonic crystal cavity and the edge of the partial photonic crystal waveguide. Here, it is worth noting that Fabry-Perot BICs have been conceived in acoustic³²⁵ and quantum systems^{326,327}.

Another type of mode interference-induced BIC is Friedrich-Wintgen BIC, which was originally proposed in quantum system¹¹⁰. According to this study, the authors unveiled that the interferences of two resonances having different channels lead to the formation of BICs. The common physical features

include the avoided crossing of the resonances' positions and the vanished linewidth for one of the resonances. Here, we want to point out that the key difference between Friedrich-Wintgen BIC and Fabry-Perot BIC is that two different modes in the same cavity are involved for the former case while the latter one arises from the coupling of two identical resonators. The formation of Friedrich-Wintgen BICs could be well described by temporal coupled mode theory. One may find mathematical derivation in other published review^{328,329}. Friedrich-Wintgen BICs not only exist in a single cavity system^{112,330} but also happen in a period structure. For instance, Azzam et al. reported that such a BIC could be found in a hybrid plasmonic-photonic system consisting of a silver grating coupled to a SiO₂ waveguide (Fig.19f-g). The rich band structures allow for observation of FW-BIC due to their destructive interferences. Lepetit et al. reported the experimental demonstration of Friedrich-Wintgen BICs in the microwave range^{331,332}. In these works, they put the high-permittivity dielectric subwavelength resonator into the metallic waveguide to mimic the wave propagation in a periodic array of resonators. The measured Q-factor is as high as 1,700. Pankin et al. successfully realized Friedrich-Wintgen BICs in the visible range with one-dimensional photonic crystals³³³. Also, Friedrich-Wintgen BICs have recently been theoretically predicted at off Γ point in a single photonic crystal slab with either a square lattice³³⁴ or a triangular lattice³³⁵. Because the fundamental physics behind FW BIC is to achieve avoided crossing of two resonances by interference, Friedrich-Wintgen BICs have been successfully reported in other wave-relate system^{112,318,325,330}.

BICs also could be linked to some interesting phenomena like zero refractive index metamaterials. Minkov et al. unveil that symmetry-protected BIC could be a zero-index mode by carefully choosing the structure parameters of photonic crystal slab³³⁶. The concept of zero-index BIC has been experimentally verified in near-infrared by Tang et al. The high-Q resonance enabled by BIC together with low loss zero index directly leads to the reduced propagation loss by order of magnitude compared to the previous design^{337,338}.

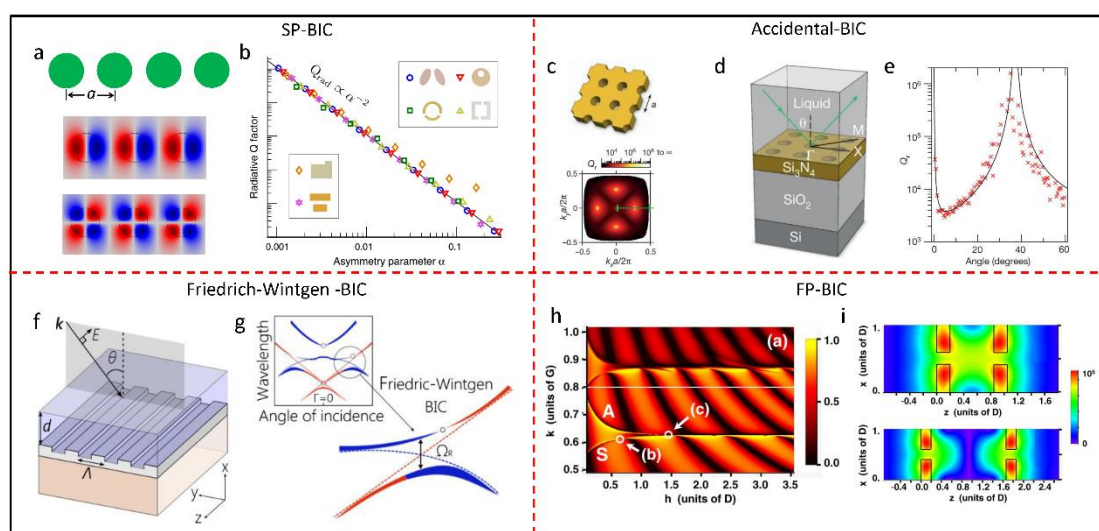


Fig.19. Four types of BICs in an array of dielectric structure. (a) Top panel is schematic drawing of circular dielectric cylinder array. Bottom panels are electric field distribution of two symmetry-protected BICs. (b) Q-factor of the metasurface with different unit cell as a function of asymmetry parameter. (c) Top panel is a schematic drawing of a photonic crystal slab. Bottom panel shows the Q-factor mapping as a function of k_x and k_y . (d) Schematic view of real photonic crystal slab with symmetric environment. (e) Numerically calculated and

measured Q-factor at different incident angles. (f-g) schematics of the hybrid plasmonic-photonic structure made of silver grating covered by SiO₂ thin film. (g) Schematic illustration of the band structure of hybrid system. (h) Reflection spectra mapping as a function of wavevector of incident wave k and the distance between two dielectric grating structures. (i) Electric field profile of two BICs in (h). (a) from Ref ²⁴. (b) from Ref ³⁰⁵. (c-e) from Ref ³¹³. (f-g) from Ref ³³⁹. (h-i) from Ref ³¹².

3.2.2 Topological Nature of BICs

Since BIC is a non-radiating eigenmode with an infinitely large Q-factor, it has vanished far-field ($E_x=E_y=E_z=0$). Fundamentally speaking, it could be assigned as a polarization singularity. Zhen et al. revealed the topological nature of BICs supported by photonic crystal slab³¹⁵. They found that each BIC could be linked to the vortex polarization singularity in momentum space. Similar to the vortex in orbital angular momentum, each BIC carries a topological charge, as shown in Fig.20a-b. The polarization vortex of BIC was experimentally verified by Doleman et al.³⁴⁰. They first identified an accidental BIC at off- Γ point in 1D Si₃N₄ grating for incidence with TM polarization by checking the vanishing resonant linewidth in reflection spectrum mapping via the angle-resolved reflection spectroscopy, and then confirmed its vortex nature by tracing the full polarization state of the far-field radiation around the BIC from the k-space polarimetry reflectivity measurements. The polarization vortex associated with BICs does exist for any periodic structure that supports BIC, such as 1D dielectric grating and 2D all-dielectric metasurface. By exploring the topological nature of the BIC-polarization vortex, Wang et al. successfully construct the optical vortex generator operating in momentum space with a single photonic crystal slab³⁴¹. Unlike the optical vortex built from the metasurface, such an optical vortex does not need to align the incident beam because the structure has no absolute centre. Also, the rich library of topological charges with different lattices (i.e. square lattice or hexagonal lattice) allows for the implementation of arbitrary order optical vortex at any wavelength. The authors fabricated a free-standing Si₃N₄ photonic crystal slab and applied the Fourier-optics-based spectroscopy technique to measure the angle-resolved spectra and transmitted light beam's profile and phase. The interference patterns shown in Fig.20i-j suggests that the generated beam is indeed optical vortices that carry topological charge $l = \mp 2$. The phase diagram indicates that the topological charges of transmitted light beam are $l=2$ and $l=-2$ for incidence with left-handed polarization and right-handed polarization, respectively.

For multiple BICs existing in momentum space supported by the same photonic array structure, see Fig.20a-b as an example, their corresponding topological charges show bouncing or annihilation but satisfy total charge conservation by changing the structure parameters. When multiple BICs merge at the same point in momentum space by carefully tuning the structure parameters (Fig.20c), a topological-protected BIC³⁴² (also called super-BIC) is formed because the Q-factor of such a BIC is more stable than normal BIC. Its Q-factor is proportional to $1/(k-k_{\text{BIC}})^4$ or $1/(k-k_{\text{BIC}})^6$ (Fig.20d) depending on the topological charge distribution compared to $Q \propto 1/(k-k_{\text{BIC}})^2$ for normal BIC, where k is the wavevector around k_{BIC} . In 2014, Bulgakov et al. found that a period array of circular dielectric waveguides could support symmetry-protected BIC and Bloch BIC at Γ point²⁴. Later, Yuan et al. applied the perturbation theory³⁴³ to prove that for the Bloch BIC its Q-factor is proportional to $1/k^4$ while symmetry-protected BIC follows $Q \propto 1/k^2$. By calculating BICs' topological charge in such a system, Bulgakov et al. found that this Bloch BIC actually is a topological-protected BICs³¹⁶. It carries a topological charge $q=0$ and arises from the merging BICs at a certain period, where two BICs along

k_x axis carry topological charges $q=1$ and the other two BICs along k_z axis have $q=-1$ if light propagates along y direction. Later, topological-protected BIC has also been constructed with an array of dielectric spheres by the same group³⁴⁴. In 2019, Jin et al. extended this conclusion to the case of Si photonic crystal slab made of an array of square lattice with cylindrical air holes³⁴². Different from the previous 1D circular grating case, it supports nine BICs, among which four BICs with $q=-1$ distribute along k_x and k_y axis, the other four with $q=1$ are located in the diagonals of four quadrants in the momentum space, and the last one is located at Γ point. Perturbation theory shows that the Q-factor of merged BICs satisfies $Q \propto 1/k^6$ when other eight BICs is shrunk towards Γ point at the same time by tuning the periodicity of lattice. Experimental results confirm that the maximum Q-factor is boosted to almost half million due to merged BIC, and Q-factor indeed decays slowly with k_x increasing compared to normal symmetry-protected BICs (Fig.20e). Besides, a more recent study shows that topological protected BIC could be induced at off Γ point³³⁴. Its formation is mainly attributed to the merging of a pair of Friedrich-Wintgen BIC with charge $q=+1$ and a pair of accidental BICs with charge $q=+1$. Since only four BICs are involved in this work, the merged BICs has a quality-factor $Q \propto 1/k^4$.

Previous discussion indicates that each symmetry-protected BIC is always accompanied by a polarization vortex carrying certain topological charges in momentum space. If the in-plane symmetry is broken in a Si_3N_4 photonic crystal slab with a square lattice of the cylindrical hole (Fig.20f-h), a pair of circular polarization states (CPSs) could be generated due to the transition from BIC to QBIC³⁴⁵, as reported by Liu et al. In 2020, two independent groups reported the polarization singularity in honey-comb photonic crystal slab^{317,346}. Yoda et al. demonstrated that high-order BIC at Γ -point that carries topological charge $q=-2$ can be split into two BICs at off- Γ point via breaking the C_{6v} symmetry³¹⁷, each of which carries the same topological charge $q=-1$. If the circular air holes are deformed into triangular air holes, C_2 symmetry is broken but C_{3v} symmetry is still preserved. Under such circumstances, six CPSs (three left-handed CPSs and three right-handed CPSs) could be spawned at off- Γ point and each CPS carries topological charge $q=-1/2$ while topological charge of BIC at Γ -point changes into $+1$. Further breaking the C_{3v} symmetry allows for observation of the generation and annihilation of CPSs with the same handedness but opposite charges. Similar conclusions are drawn in another work done by Ye et al.³⁴⁶, where they focus on Dirac-degenerate points and BICs at K point in the first Brillouin zone, CPSs. Instead of breaking the in-plane symmetry, Yin et al. introduced the out-of-plane symmetry broken for 1D Si grating to achieve unidirectional guided resonances³⁴⁷. A pair of half-integer topological charges are created due to up-down mirror symmetry. They evolve in momentum space and bounce into each other with the angle of the sidewall decrease. Only when these two half-integer charge merges again as an integer charge, downward radiation is significantly suppressed due to the vanished far-field of BIC nature. Consequently, ideal single-side radiation is achieved. They also experimentally demonstrated this new type of guided resonance that enables single-side radiation, whose Q-factor is up to 1.6×10^5 . Its topological nature is confirmed by far-field polarimetry measurement.

Since there are rich polarization properties around BICs, BIC has been demonstrated as a versatile platform to tailor the wavefront of circularly polarized light in a nonlocal way. By introducing different types of perturbation on the unit cell, Overvig et al. successfully demonstrated multifunctional nonlocal metasurfaces that allow for manipulating the wavefront of circularly polarized light (i.e. focusing) at single or multiple BIC resonances³⁴⁸. Moreover, chiral perturbation-induced QBIC could help to build

arbitrary elliptical polarization³⁴⁹, leading to the observation of spin-selective Fano resonance metasurface with near-unity efficiency. Later, the same group developed a general concept of Fano resonance based on symmetry-protected BICs. Unlike conventional Fano resonance only operating in the momentum-frequency domain, the generalised Fano resonance could be selectively excited in the space-frequency domain and allows for tailoring the light in multidimensions³⁵⁰, such as frequency, polarization and wavefront. Besides, the chiral effect born of QBIC makes it possible to maximize the chirality at resonance, as theoretically demonstrated by Gorkunov et al.³⁵¹

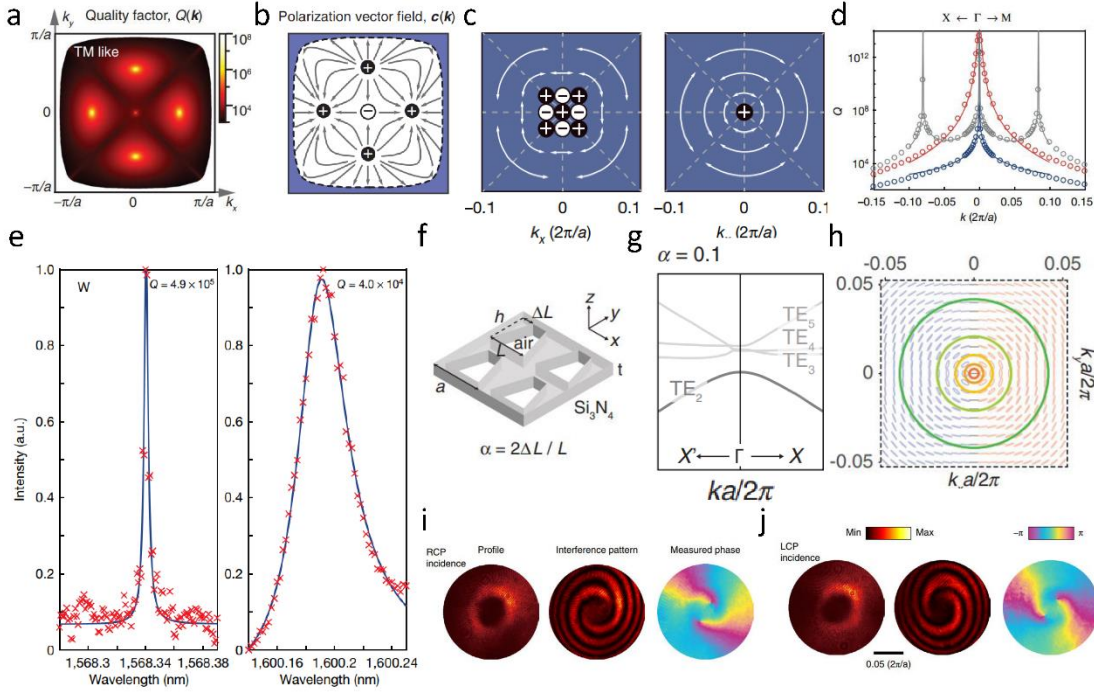


Fig.20. Topological property of BIC and its applications. (a) Q-factor mapping vs (k_x, k_y) . (b) Plot of polarized vector field. (c) Merged BICs through structure parameter engineering. (d) Q-factor of eigenmode without and with BIC merging. (e) Left panel is the measured scattering spectrum of photonic crystal slab supporting merged BICs. Right panel is the measured scattering spectrum for normal symmetry-protected BICs. (f) Schematic view of photonic crystal slab with deformed hole shape. (g) Band structure of photonic crystal slab with asymmetry parameter $\alpha=0.1$. (h) Polarized vector field distribution. (i-g) Optical vortex beam generation by BIC supported in photonic crystal slab. (a-b) from Ref ³¹⁵. (c-e) from Ref ³⁴². (f-h) from Ref ³⁴⁵. (i-j) from Ref ³⁴¹.

3.2.3 Multipolar Origin of BIC

Except for topological interpretation, the formation mechanism of BIC has been revealed by multipolar analysis approach. Sadrieva et al. conducted a thorough study on unveiling the fundamental physics of both symmetry-protected BIC and accidental BICs in an all-dielectric metasurface by performing the multipole decomposition³⁵². For a two-dimensional array of dielectric meta-atoms in xoy plane, they found that symmetry-protected BIC at Γ point are the superposition of several multipoles that have nonradiation along the z axis (Fig.21a). In other words, all other multipoles could be included except for Y_{pmn} with $m=1$ because only the channel with $m=1$ shows radiation along z axis. However, accidental BIC at off Γ -point is ascribed to the destructive interference of multipoles in the far-field (Fig.21a). Later, Chen et al. established a subtle correlation between multipolar singularity indices and the topological charge of BICs by mapping the radiation singularities to the open radiation channels³⁵³

(Fig.21b-d). With these multipole informations, let us revisit the all-dielectric metasurface that supports BICs. The lowest-order BIC in an array of dielectric nanodisks belongs to magnetic dipole BICs with magnetic moment perpendicular to the cross-section of disk. Due to dark mode nature of this BIC, one has to bring perturbation into the meta-atoms to break the symmetry by either introducing an off-centre hole inside or removing an arc from the whole disk^{292,293,303,304}. The rich multipolar properties of BICs also bring much freedom in designing metasurfaces. For example, He et al. found that a toroidal BIC could be achieved by replacing the meta-atom in the array structure with a cylinder nanodisk dimer³⁵⁴. Another way of realising toroidal BICs is to introduce a hole or a slit inside the nanodisk array^{355,356}, as independently reported by Liu et al. and Algorri et al. It is worth pointing out that the symmetry in the single unit cell is preserved, and toroidal BICs only happen at certain parameters. The evolution from BIC to QBICs is enabled by either changing the period or the hole size. More interesting thing is that toroidal QBICs are able to be excited at normal incidence without breaking the structure symmetry. Following these design strategies, Jeong et al. successfully realize a high-Q toroidal resonance, whose Q-factor is up to 728 at 1505nm³⁵⁷. Given the rich physics of the multipolar effect and their connection with BICs, we expect that more BICs with unique multipolar properties can be found, and in turn they may help to tailor the far-field radiations.

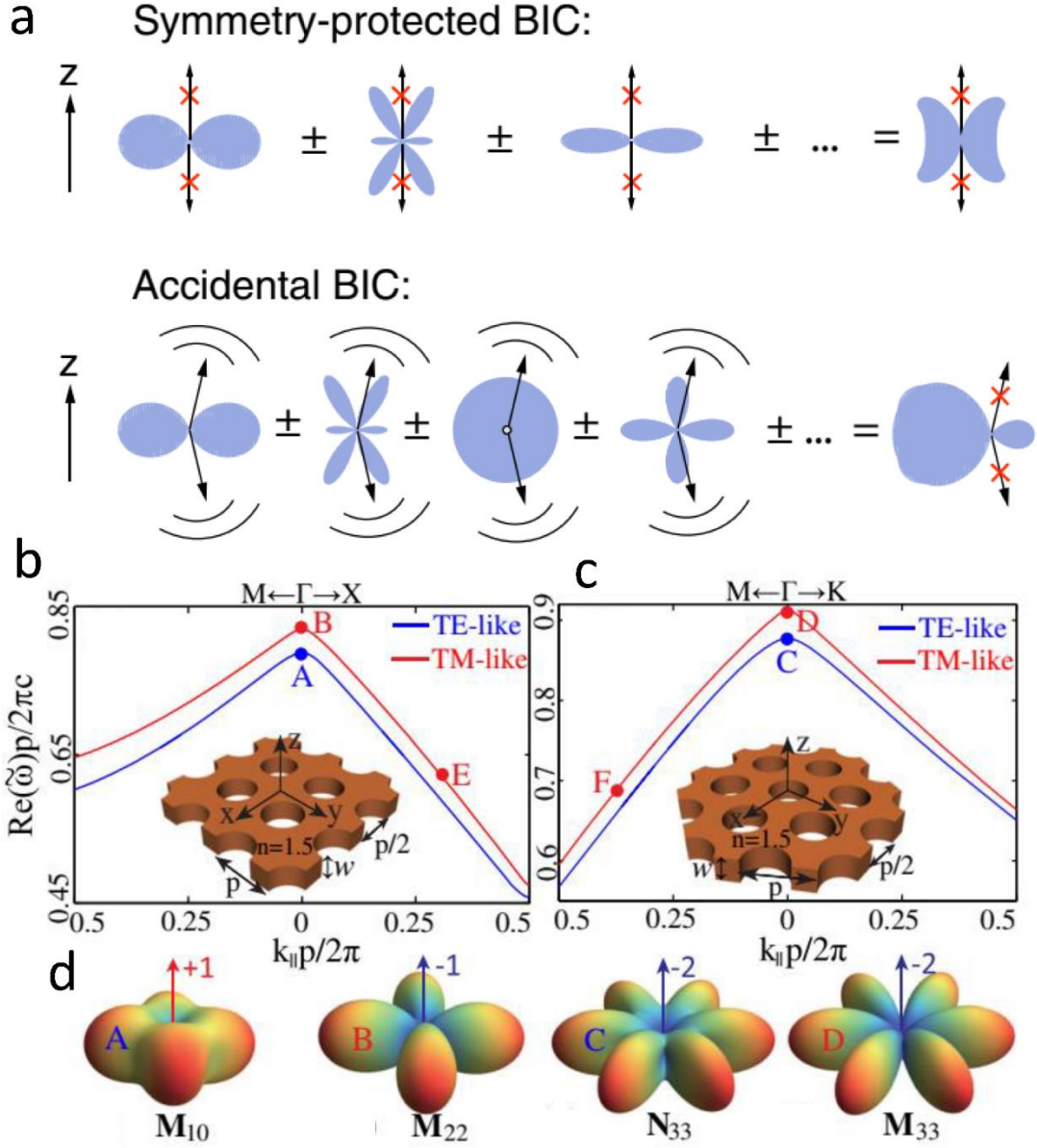


Fig.21. Multipolar property of BIC (a) Schematic illustration of symmetry-protected BIC and accidental BIC formation mechanism. (b-c) band structure of photonic crystal slab with square lattice and honeycomb lattice. (d) Multipolar radiation pattern for four BICs at Γ point. (a) from Ref ³⁵². (b-d) from Ref ³⁵³.

3.3 Applications of BICs in enhanced light-matter interactions

As the essence of BIC is a leaky mode with an infinitely high-Q factor falling within the continuum spectrum, the emergence of BIC is always accompanied by extreme field enhancement at resonant wavelength. This unique property makes BIC attractive for enhancing light-matter interactions, such as light emission, absorption, nonlinear harmonic generation, strong coupling, sensor, etc. However, an ideal BIC corresponds to an optical resonant mode with zero radiative decay rate (or infinitely long radiative lifetime). It could not be coupled with external excitation. Thus, in real applications, the conversion from BIC into quasi-BIC has to be made by introducing the tiny perturbation (i.e.,

symmetry-broken) such that such high-Q modes could be excited with different types of incident wave, such as plane wave and vector beam. In the following sections, we review the recent progress of BIC in enhancing light-matter interaction.

3.3.1 BIC for Enhanced Light Emission and Lasing

As discussed in the previous section, the key to realising enhanced light emission is to place the emitter into an optical cavity that confines the electric field into a small volume. As a peculiar cavity mode, BIC that simultaneously enables an ultra-high-Q factor and strong field localization, has been widely used to boost the light emission and realising laser with an ultralow threshold. Two groups independently reported the giant enhancement of PL intensity by quasi-BIC mode when the quantum emitters are embedded in an all-dielectric metasurface with the broken-symmetry^{358,359}. Yuan et al. experimentally demonstrated that PL intensity of Ge QDs could be enhanced by three orders with asymmetric silicon metasurface³⁵⁸. The asymmetry is created by transforming a circular hole into a hole with a half-circle and a half-elliptical shape. The measured Q-factor of QBIC is up to 1011. Later, Liu et al. reported a 110-fold enhancement of PL from InAs QDs that are integrated with the III-V metasurfaces³⁵⁹. Such a large enhancement factor is attributed to the excitation of out-of-plane MD-QBIC mode with high-Q factor by breaking the symmetry of Mie-resonator, where a corner is removed in the GaAs cuboid unit cell. Besides, the far-field divergence was reduced significantly owing to the coupling between in-plane and out-of-plane dipole modes. Here, it is noteworthy that although the Q-factor is reasonably high, lasing does not happen in these two cases because the quantum yield of InAs QDs and Ge QDs is relatively low.

Previous discussion has shown that a single dielectric NP supports high-Q QBIC modes, lasing in a subwavelength dielectric NP becomes accessible when QBIC mode is combined with gain materials with high quantum yield. Mylnikov et al. presented the first experimental demonstration of such a nanolaser operating at 825nm based on a subwavelength GaAs nanocylinder³⁶⁰(Fig.22a-c), which has a height of 330nm and a diameter of 500nm. The threshold is around 300uJ/cm², larger than the counterpart of lasing in an array structure because the lasing Q-factor is 235, almost one-order lower than the Q-factor of QBIC in an array of GaAs nanoantenna. Besides, this laser can only operate at low temperatures (77K), this issue may be overcome by considering high-gain materials. However, one must keep in mind that the Q-factor of QBIC in a single nanostructure highly depends on its refractive index. As such, materials with high-index and large gain-coefficients are required to realize low-threshold laser at room temperature. Apart from QBIC-based lasing, Yu et al. demonstrated a Fano BIC lasing based on a photonic crystal cavity coupled to a terminated waveguide³²⁴ (Fig.22f-g). As discussed in the previous section, the physical nature of such a BIC is mirror-induced Fabry-Perot BICs. Compared to the laser enabled by the L7 photonic crystal cavity, where the gain medium is embedded into the cavity region, the authors put active materials inside the continuum region. This significantly reduced the loss and improved the effective Q-factor of the system. Consequently, emitted photons from the active region could be stored in the cavity region for a longer time and the line width of such a Fano laser is much less than that of a conventional photonic crystal cavity.

Lasing action with BICs has also been implemented in periodic systems like photonic crystal slab and dielectric metasurface. In fact, lasing with symmetry-protected BIC is not new. It could be traced back to more than two decades ago and was recognised as a photonic crystal surface-emitting laser (PCSEL)

operating at gamma-point. Compared to the photonic crystal cavity-enabled laser, such a PCSEL can operate in a large area^{361,362}. For example, the Noda group from Kyoto university successfully realized PCSEL in near infrared³⁶³ and blue-to-violet wavelength range³⁶⁴. Also, the output power of single-mode PCSEL could be improved to Watt class by exciting a QBIC with asymmetric triangle hole array³⁶⁵, as demonstrated by Hirose et al. The record of PECSEL output power has been broken in 2019 by employing a double-lattice photonic-crystal resonators³⁶⁶. In this study, one lattice is shifted by one-quarter wavelength along both x and y directions with respect to another so that the oscillation of high-order modes is suppressed by more than one-order of magnitude compared to conventional design. With the optimised double-lattice photonic-crystal resonators, the output laser power was boosted to 10W under the pulse excitation. Additionally, such a laser has a large emission area with a diameter of 500um and an ultra-narrow divergence angle ($<0.3^\circ$). Even for continuous pumping, the maximum laser power is as large as 7W. Later, such a double-lattice structure was used to realize PCSEL with arranged gain and loss section in two-dimensional configuration³⁶⁷, where the peak power is up to ~20W and pulse width is as short as ~35s with an injection current of only 3-4A. One may consult more research on PCSEL in a review written by Noda et al.³⁶⁸.

Another example of BIC-enabled lasing was reported by Zhen et al.³⁶⁹. In this study, lasing is attained with a threshold as low as $9 \times 10^3 \text{ nJ/cm}^2$ when a 100nm organic molecules (Rhodamine 6G) solution was suspended onto a photonic crystal slab that supports symmetry-protected BIC. Kodigala also reported a room temperature laser at around 1550nm from an optical pumped BIC cavity that is made of an array of cylindrical nanoresonator³⁷⁰ (Fig.22d-e). In this work, $\text{In}_x\text{Ga}_{1-x}\text{As}_y\text{P}_{1-y}$ multiple quantum well is patterned and suspended to create a BIC mode at 1550nm. It is worth pointing out that such a resonance-trapped BIC belongs to a topological BIC because its Q-factor decays slower with k-vector than the symmetry-protected BIC. The BIC could be made by fine-tuning the radius of the cylinder resonator without resorting to symmetry-broken. Single mode Lasing at 1551.4nm was experimentally confirmed in a 16×16 nanoresonator array by checking the output power as a function of pumping power and wavelength, as shown in Fig.22e. Due to the high-Q-factor enabled by QBIC, the threshold power is as low as $56 \mu\text{W}$. It is interesting to note that lasing behavior persists even in a 8×8 nanoresonator array because a large Q-factor is still maintained in such a finite structure. This finding suggests a viable way of realising laser with relatively small size.

Besides, the rich far-field property of BIC makes directional lasing possible. By utilising the vertical electric dipole BIC supported by a dielectric nanoantenna array, Ha et al. realized directional lasing with GaAs nanopillar array³⁷¹. One of the periods for GaAs photonic lattice is tuned to open a leaky channel so that the ideal BIC is transformed into QBIC, where a high-Q value is still maintained after such a transition. The threshold is only $14 \mu\text{J/cm}^2$ due to the high lasing Q-factor 2,750 at 825nm, which is retrieved by retrieving the reduced full-width-half-maximum 0.3nm. Also, the vertical dipole nature leads to the directional emission at 3° . The emission angle can be tuned to even 25° by exciting high-order modes, but the price is the reduced Q-factor. Also, it should be pointed out that although tunable laser wavelength is demonstrated by tuning the working temperature, the poor quantum efficiency makes the laser operate at a relatively low temperature. Later, many efforts were devoted to elevating the laser operating temperature to room temperature. Instead of directly patterning the thin film made of gain materials, Wu et al. demonstrated a magnetic dipole (MD)-BIC-enabled laser at room temperature by coating a thin layer of colloidal CdSe/CdZnS core-shell nanoplatelets onto a square lattice of TiO_2 cylinder³⁷². Benefiting from the ultrahigh-Q factor of BIC mode, the threshold is

as low as $36\mu\text{J}/\text{cm}^2$ when the resonant wavelength of high-Q mode is perfectly matched the peak of PL from thin-film gain materials. Also, this BIC has a nature of out-of-plane magnetic dipole, thus enabling a single-mode laser with an ultrasmall divergence angle of 0.8° . More recently, the same group applied the concept of BIC to realize the lasing with colloidal quantum-dots (CQD)³⁷³. Symmetry-protected BICs are formed by coupling slab waveguide modes in planar CQD film to the TiO_2 nanoantennas array. Thanks to the ultrahigh-Q factor of BICs modes, ultralow threshold $11\text{kW}/\text{cm}^2$ is attained under 5-ns pulse laser pumping. Since a square array of TiO_2 nanocylinder supports multiple symmetry-protected BIC at Γ point, Azzam et al. experimentally demonstrated single and multi-mode directional lasing by spin-coating polyvinyl alcohol (PVA) solution of an organic gain medium (Rhodamine 101) on top of TiO_2 NP array³⁷⁴. Yang et al. implemented hybrid surface lattice resonance to construct BICs in Si_3N_4 metasurface³⁷⁵. By coating rhodamine 6G onto the metasurface, they realize a directional laser with an ultralow threshold and high coupling factor at room temperature. To further shrink the footprint and reduce the laser threshold, Hwang et al. utilised the super-BICs arising from the merged BICs in the momentum space³⁷⁶. Experiment measurements showed that the threshold decreased to $1.47\text{ kW}/\text{cm}^2$ even with a finite-sized photonic cavity. An interesting finding in this work is that optimum lattice constants happened at pre-merging BICs instead of merging BICs due to mode broadening in finite-size photonic structures.

Note that all of the previous designs rely on the reactive ion etching, laser also could be achieved in an etchless way³⁷⁷, as demonstrated by Wang et al. In this study, perovskite is used as a gain material due to its high quantum yield. Symmetry-protected BIC is realized by simply patterning the low-index polymer layer (i.e. photoresist like ZEP520A) onto continuous perovskite thin film. The marriage of perovskite and symmetry-protected BIC ensures a single-mode laser with a simultaneous ultralow threshold $49\mu\text{J}/\text{cm}^2$ and a small divergence angle $<1^\circ$ in the far-field. Also, lasing at different wavelengths is easily obtained by merely changing the width of polymer grating while the threshold power is maintained around $50\mu\text{J}/\text{cm}^2$. Here, it is worth commenting that all reported BIC-based lasers so far are achieved by optical pumping, it is necessary to develop an electric-pumping laser by injecting carriers to the whole cavity region. Also, the lasing wavelength could be easily tuned by either putting the cavity on the flexible substrate or employing electro-optical effects.

Because each BIC in the extended photonic system corresponds to the vortex singularity that carries a topological charge, this provides an alternative solution for realising the vortex laser³⁷⁸. By taking advantage of symmetry-protected BIC with topological charge +1, Huang et al. experimentally demonstrated a vortex laser in an all-perovskite metasurface with schematic drawing shown in Fig.22h. The lasing behavior is verified by the evolution of emission spectrum at different pumping densities. The vortex emission is indicated by the doughnut-shape of the far-field pattern measured by back-focal plane imaging technology. The radial polarization is also confirmed by checking the far-field pattern after putting a linear polariser behind the doughnut beam, where two-lobes is always observed with the polarization rotating exactly following the direction of linear polarization. Besides, the exceptional gain coefficients of perovskite allow for converting such a symmetry-protected BIC into QBIC via locally pumping the metasurface. For example, by transforming the pumping region from circle to ellipse, the far-field pattern changes from a doughnut-shape to two lobes (Fig.22i), indicating the transition from vortex laser to linear polarized laser. A similar phenomenon is also observed by applying two pumping beams onto a shifted area. Furthermore, they also demonstrated temporal control on the polarization switching from vortex to linear polarization and vice versa. The transition time is as short as 1-1.5s. Also, the high-Q factor of QBIC and large gain coefficient together contribute to an order magnitude

reduction of energy consumption compared with the other design. It is noteworthy that a high-order vortex beam could be generated by employing high-order BIC supported by photonic crystal slab^{379,380}. We should expect that the vortex beam family could be expanded by using different photonic lattice arranges like square lattice and hexagonal lattice that supports both low and high-order BICs. This may hold great promise in optical communications. More recently, by taking advantage of chiral-BICs, circular polarized lasing has been demonstrated experimentally with resonant metasurfaces without involving spin injection³⁸¹.

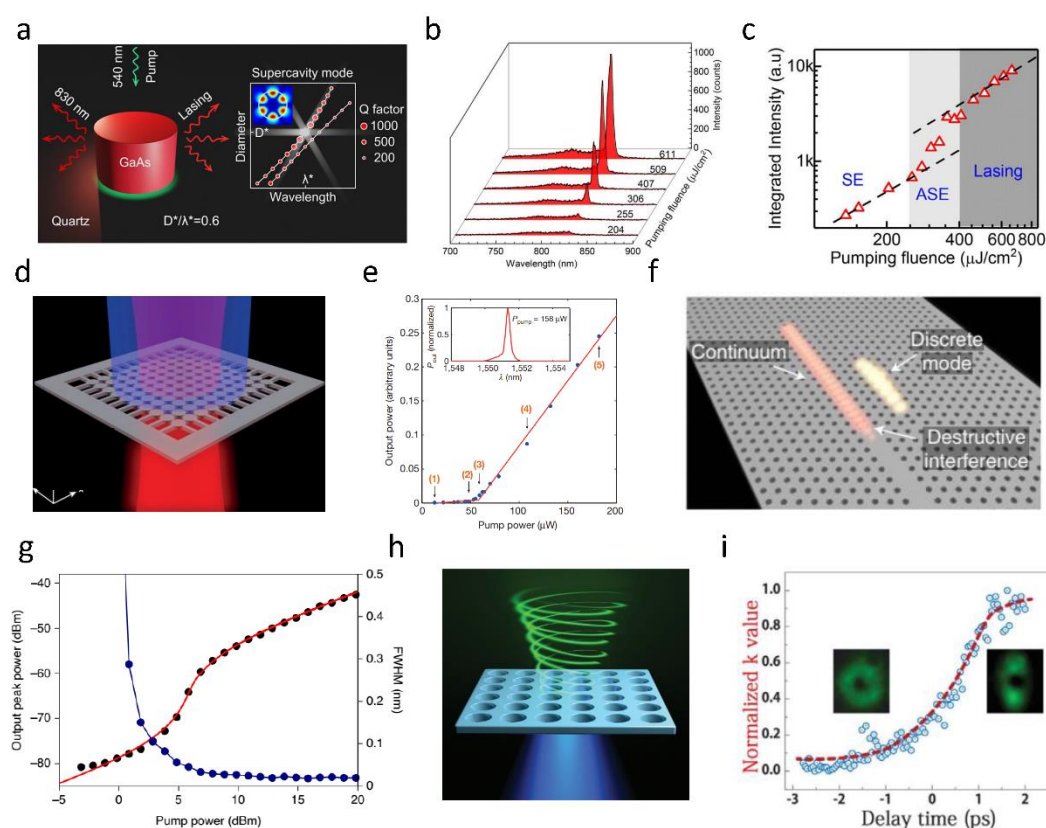


Fig.22. Lasing in BIC. (a) Schematic illustration of QBIC enabled Lasing in a single GaAs cylinder resonator. (b) PL spectra at different pumping power. (c) log-log plot of emission intensity as a function of pumping fluence. (d) Schematics of lasing in a freestanding InGaAsP metasurface. (e) Emission power as a function of pumping paper. (f) Schematics of Fano BIC laser. (g) Output peak power and FWHM as a function of pump paper. (h) Schematic drawing of BIC-enabled vortex microlaser based on perovskite metasurface. (i) Temporal evolution of BIC lase. (a-c) from Ref ³⁶⁰. (d-e) from Ref ³⁷⁰. (f-g) from Ref ³²⁴. (h-i) from Ref ³⁷⁸.

3.3.2 Enhanced Nonlinear Harmonic Generation

As discussed above, leaky modes with infinitely large Q-factor, also called quasi BICs in subwavelength resonators, can be obtained by suitably modifying geometrical parameters of the subwavelength resonators, such as tuning the size ratio, to overlapping two or more modes both spectrally and spatially. This provides a promising route to realize strong scattering and absorption efficiencies from subwavelength resonators. These leaky modes can be excited directly by external light illumination, and they enable packing electromagnetic energy at the subwavelength scale with strong electric and magnetic near-field enhancement inside the cavity or near the surface of the cavity, and thus can significantly boost the light-matter interactions from the cavity. In recent years, these

supercavity modes further motivated the applications of subwavelength resonators in nonlinear optics, and offered a paradigm shift in nonlinear optics. Inspired by the concept and mechanism, researchers have explored various nonlinear effects from subwavelength resonators based on materials with high nonlinearities, including Si for third-order nonlinear processes, and III-V semiconductors for second-order nonlinearities.

BICs From Individual Subwavelength Resonators

The study of individual subwavelength resonators has been continuously triggering extensive interest due to their ability to realize nonlinear emitters with a subwavelength scale which is highly beneficial for on-chip source elements. For an individual resonator, the formation of supercavity modes can be understood through the multipolar transformations of coupled leaky modes. The BIC appears with increasing the order of the dominating multipole, where lower-order multipolar losses are completely suppressed. This will further lead to a high Q-factor of the mode associated with strong electromagnetic field confinement for boosting nonlinear light-matter interactions³⁸². In 2018, Carletti et al. designed a subwavelength dielectric AlGaAs resonator supporting high-Q supercavity modes, and further excited it using an azimuthally-polarized pump to enhance the second-harmonic generation. As a result, a record-high conversion efficiency of the SHG has been theoretically predicted, i.e., the conversion efficiency of SHG exceeds two orders of magnitude of the conversion efficiency observed when pumping at the magnetic dipole Mie resonance³⁸³. Later, they further combined the concept of BIC with smart engineering of the substrate that undergoes a transition from an insulator to a conductor via an epsilon-near-zero (ENZ) regime, to theoretically explore the high-harmonic generations based on the Silicon resonators, including third-harmonic generation, degenerate four-wave mixing, and cascaded harmonic generations³⁸⁴. It has been shown that by the engineering of the substrate, at the quasi-BIC regime, the Q-factor of supercavity mode supported from individual subwavelength resonators can increase from the previous 110 to more than 310, and a significant electric near-field enhancement of 200 has been realized theoretically. These substantially induce strong nonlinear effects at the nanoscale. Such individual dielectric nanoresonators supporting high-Q leaky modes were realized experimentally in 2020 using AlGaAs nanodisks placed on an engineered three-layer substrate (SiO₂/ITO/SiO₂) as shown in Fig.23a-c³⁸⁵. Under the excitation of an azimuthally polarized cylindrical vector beam, a Q-factor of 190 has been experimentally obtained by adjusting the thickness of the SiO₂ and ITO layer. The experimental results further demonstrated a significant enhancement of SHG in the vicinity of the leaky mode (Fig.23b). An SHG efficiency exceeding $10^{-6}W^{-1}$ from the individual AlGaAs subwavelength resonator is experimentally obtained, which is more than 2 orders of magnitude higher than the efficiency when pumping at the dipole resonance (Fig.23c). A further combination of leaky mode in special optical resonators in the presence of gain and loss has demonstrated a sharp increase in the Q-factors, and a theoretically predicted SHG efficiency of 4.82×10^{-2} is obtained³⁸⁶.

BICs From Metasurfaces

Metasurfaces have been served as a robust platform for shaping nonlinear emissions. High-Q leaky modes supported in metasurfaces play a critical role here. One typical type of them is formed by the bound state of one symmetry class embedded in the continuum spectrum of another symmetry class. Modes of different symmetry classes are completely decoupled and form strongly bound states with no radiating, which are also called symmetry-protected BICs. Researchers have employed this concept to

design high-Q leaky modes from silicon metasurfaces to enhance the third-order nonlinear responses, such as high-Q leaky mode based on longitudinal magnetic dipole resonance in silicon metasurfaces³⁸⁷. MD is well known for its ability to obtain large near-field enhancement and large mode volume compared to other multipoles and has already been widely used to enhance nonlinear generations. Employing the leaky mode theory to design a high-Q MD leaky mode in a silicon nanoblock metasurface can significantly enhance the third-harmonic generation (Fig.23d-f)³⁸⁷. Other shapes of metasurfaces, such as the nanodisk and nanobar metasurfaces, have also been employed to realize the high-Q leaky mode for nonlinear generation applications^{293,297,388,389}. GaP material has recently been employed to design a high-Q leaky mode for second-harmonic generation. Anthur et al. have successfully obtained second-harmonic generation efficiencies³⁹⁰ around $5\text{e-}5\%W^{-1}$ from a GaP metasurface when pumping with a NIR continuous light wave at a wavelength of 1200 nm and intensities of 1kW/cm^2 . QBICs have also been harnessed to enhance another quantum process-spontaneous parametric downconversion. By leveraging their high-Q factors and excellent field confinement, the emission of the nondegenerate entangled photon was greatly boosted with resonant nonlinear metasurfaces³⁹¹.

The induced light trapping and intense field at the resonance of the leaky mode from individual resonators or dielectric metasurfaces help to enhance the nonlinear responses from the host itself and enhance the nonlinear response from the adjacent materials or structures. For example, integrating 2D materials on silicon metasurfaces supporting high-Q leaky modes brings the nonlinearity associated with 2D materials into silicon photonics. The effective nonlinear susceptibility of a WS_2 monolayer can be boosted dramatically by placing it on top of a Si metasurface supporting high-Q BICs (Fig.23g-i). As shown in Fig.23h, a WS_2 monolayer combined with a silicon metasurface hosting BICs exhibits SHG intensity enhancement by more than three orders of magnitude as compared to a WS_2 monolayer on top of a flat Si film of the same thickness²⁹⁸. MoS_2 monolayer and few-layer GaSe flakes, have been coupled into high-index dielectric metasurface supporting high-Q leaky modes and demonstrated giant nonlinear emissions^{392,393}.

Besides the nonlinear emission intensity enhancement, nonlinear wave control has been another important research direction. By designing a high-Q leaky mode on a metasurface based on chiral broken-symmetry, it can selectively excite this mode under the illumination of particular light polarization, and further, attain nonlinear circular dichroism³⁹⁴. For high-Q leaky mode in a metasurface, asymmetric field enhancement can be obtained by controlling the asymmetry parameter of the metasurface, this further can be used to generate giant asymmetric nonlinear emissions with high efficiency^{395,396}.

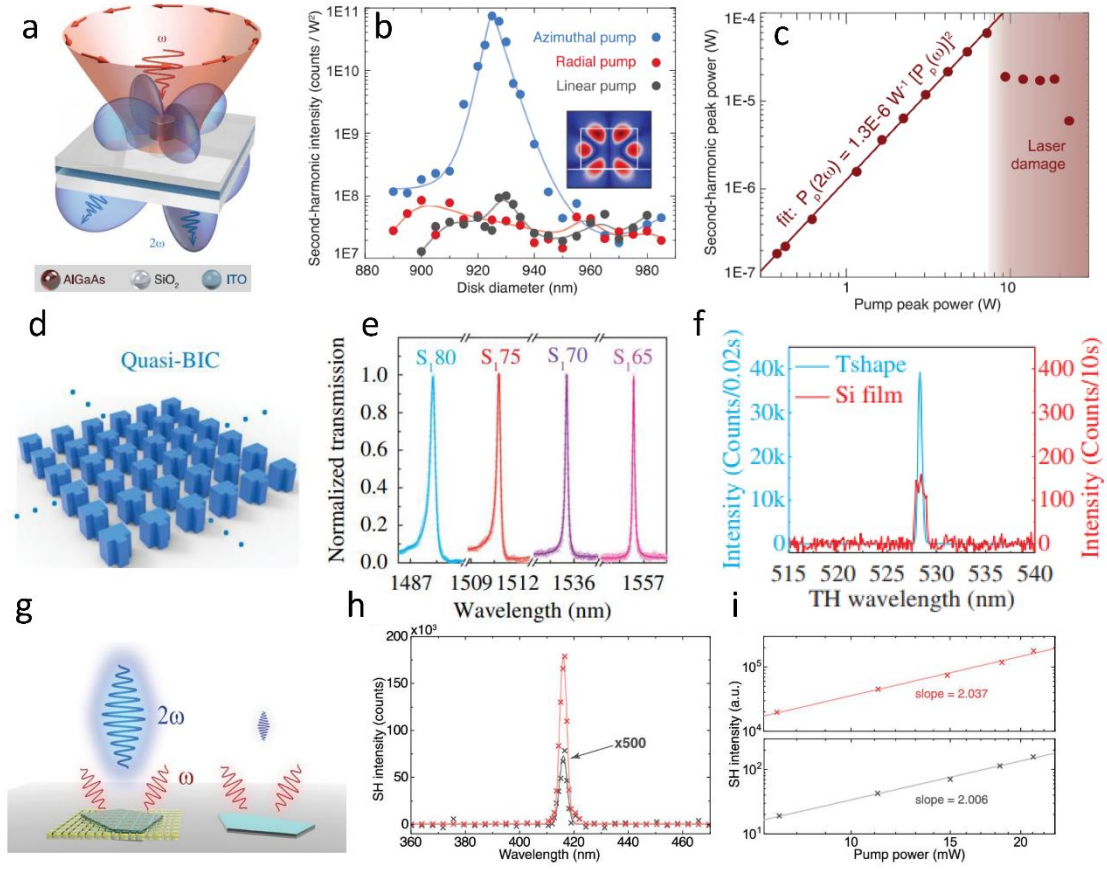


Fig.23. Nonlinear enhancement from dielectric nanostructures driven by BICs. (a-c) SHG from a AlGaAs QBIC nanoantenna. (a) Schematic illustration of the SHG in an AlGaAs nanoresonator under azimuthally polarized vector beam excitation. (b) Measured SH intensity as a function of the nanoresonator diameter for different pump polarizations. The inset shows the near-field profiles at the QBIC. (c) Measured peak SH power versus the peak pump power for a nanoresonator with a diameter of ~ 930 nm. (d-f) Enhanced THG from a high-Q QBIC Si metasurface. (d) Si metasurface with symmetric defects that supports quasi-BICs. (e) The calculated transmission spectra of 21×21 Si blocks with different defect sizes. (f) Comparison of the THG in quasi-BIC metasurface and a reference Si thin film with the same thickness as the metasurface. (g-i) Illustration of enhanced SHG from 1L WS₂ combined with a Si metasurface hosting BICs. (g) Illustration of the SHG from 1L WS₂ with and without the quasi-BIC Si metasurface. (h) Measured SH intensity spectra from WS₂ monolayers on top of the optimized quasi-BIC metasurface (red) and on top of the reference bulk Si film (gray). (i) Measured SH intensities vs the pump power for WS₂ monolayers on top of the metasurface (red) and bulk Si film (gray). (a-c) from Ref ²⁷⁸. (d-f) from Ref ³⁸⁷. (g-i) from Ref ²⁹⁸.

3.3.3 BIC for Biosensor and Filter

Optical sensors can detect the refractive index change of background medium from light absorption and scattering spectrum³⁹⁷. As a noninvasive technique, optical sensing relies on the optical resonance that is highly sensitive to the refractive index change. The most widely used optical sensor is based on surface plasmon resonance or localised surface plasmon resonance. Since the electric field of surface plasmon resonance is confined at the interface of metallic NPs, even a tiny refractive index change of the background medium could induce a remarkable resonance shift. However, their performances are still limited by the low-Q factor of plasmonic resonance arising from the considerable intrinsic loss.

Bound state in the continuum supported by the all-dielectric metasurface made of an array of subwavelength nanoresonators provides a nice solution for high-performance optical sensors because it exhibits both ultrahigh-Q-factor and giant field enhancement. In this section, we review the recent progress of BIC-based sensors.

Tittl et al. reported a mid-infrared nanophotonic sensor with all-silicon metasurfaces²⁹⁹. In their design, a silicon dimer with two elliptical cylinders is chosen as the unit cell of metasurface for the following two reasons. First, such an array structure supports a BIC or QBIC when the angle between silicon dimers is zero or nonzero. The Q-factor of QBIC could be tailored by tuning the angle of two Si nanocylinders. Second, the electric field is strongly localized around the edge instead of inside of the dielectric nanostructure. This makes the high-Q mode quite sensitive to the background medium. The resonant wavelength is tuned to cover a broadband wavelength range from 1350 to 1750cm⁻¹ by simply scaling the unit cell. The real optical sensor is made of an array of 10×10 metapixels, each of which consists of a silicon metasurface providing the desired high-Q resonance. Such a configuration establishes a one-to-one correspondence between spectrum position and spatial information and enables barcoding imaging. Thus, chemical molecules adhered to the metasurface could be easily identified by simply comparing the barcode-imaging from metapixels. The large Q-factor with an average value >200 pushes the detection limit to 2130 molecules/μm², one-order of magnitude better than the sensor based on metallic nanoantenna. Later, the same group develop another type of high-Q metasurface sensor³⁰⁰. Instead of using pixelated metasurfaces, only a single Ge metasurface made from the same unit cell has been used (Fig.24a-c). This work explored the high-Q resonance across the mid-infrared wavelength range from such a metasurface by varying the incident angle. As shown in Fig.24d, it can be found that 200 high-Q resonances are created from 1100cm⁻¹ to 1800cm⁻¹ by changing the angle of TE and TM incidences. After spin-coating a thin layer of PMMA on top of metasurface, both the resonant wavelength and amplitude of the reflection peak are modulated, as seen in Fig.24e. The absorption of PMMA is retrieved as $A(\theta)=\log(R_A(\theta)/R_0(\theta))$ (Fig.24f), where $R_0(\theta)$ and $R_A(\theta)$ are the reflectance at each angle before and after polymer coating. The excellent performance of the metasurface-based sensor has been confirmed by comparing it with standard infrared absorption spectroscopy. Following the same design strategy, in 2019, Yesilkoy et al. developed an ultrasensitive hyperspectral imaging technique for label-free biosensing that operates in the near-infrared based on all-dielectric high-Q metasurface³⁰¹. The experimental results reveal that the detection limit has been pushed to less than three molecules per μm². Two years later, the same group took one step further and developed a single wavelength imaging biosensor that detects the extracellular vesicles spatially and temporally³⁹⁸.

Except for sensing molecules by measuring their vibration modes across a broadband wavelength range, the optical sensor also could detect the tiny perturbation from the environment by measuring the resonant peak shift. Usually, the performance of optical sensor is evaluated by the bulk sensitivity $S=\Delta\lambda/\Delta n$ and figure of merits $FOM=S/FWHM$, where FWHM is full width at half maximum. Typically, a high-Q factor is necessary to obtain a large FOM. Thus, QBIC exhibiting a high-Q factor is a perfect candidate for realizing high-performance optical sensors. Romano et al. experimentally realized a sensor with bulk liquid sensitivity of 178nm/RIU and FOM up to 445 by exploiting a QBIC ($Q\approx 2,000$) in photonic crystal slab³⁹⁹. Such a sensor also detects ultralow-molecular-weight molecules, where a 6nm resonance shift could be induced by less than 1nm thick molecular layer. Wang et al. demonstrated a biosensor based on a silicon crescent metasurface. Such a metasurface simultaneously first-order and high-order QBICs. Experimental results showed that the high-order BICs have better

sensitivity up to 326 nm/RIU than the first-order BICs⁴⁰⁰. All-dielectric metasurface-based sensors' performance could be further improved by employing an evanescent field sensing of BIC⁴⁰¹. In this case, the sensitivity shows an exponential increase with the cladding refractive index. Theoretical calculation indicates that the maximum sensitivity is almost 4000nm/RIU. A more advanced sensing technique called cavity-enhanced hyperspectral refractometric imaging was proposed with a single layer of photonic crystal slab⁴⁰². The operating principle is to explore the surface-enhanced fluorescence and refractometric imaging with two high-Q resonances arising from two QBICs. Such as double high-Q-resonance-based imaging leads to a resolution of 10^{-5} RIU. The superior performance of the dual-BIC-enabled sensor is verified by refractometric imaging of a live PC3 cell shown in Fig.24g-i. Bright field microscopy image, as shown in Fig.24g, is also taken to make a comparison. Finer details of the cell can be resolved by this sensor. Other structures are also proposed to realize sensors operating in terahertz^{403,404}, visible⁴⁰⁵, and near-infrared wavelength window⁴⁰⁶.

High-Q resonance from QBIC also allows for molar chiral sensing. Many biomolecules and drugs have left and right-handed forms, also called enantiomers. Different handedness leads to diverse functionality, and thus it is of vital importance to characterize the chirality. Typically, the chirality of molecules can be detected by shining light on the structure. It could be evaluated by the optical chirality, which is defined as $C = -k_0/2c \text{Im}(E^* \cdot H)$. Here k_0 and c are the wavenumber and speed of light, respectively, E and H are complex electric and magnetic fields. QBIC provides a perfect platform for boosting optical chirality because it can induce a giant electric and magnetic field around the structure when a proper BIC is chosen. A theoretical study found that by taking advantage of QBIC supported by a PbTe metasurface the optical chirality is improved to 270 in mid-IR. Later, another theoretical work demonstrated that high-Q resonance governed by QBIC could be used to measure the molar concentration of chiral molecules⁴⁰⁷. On the one hand, the large field enhancement arising from high-Q resonance leads to the increase of optical chirality. On the other hand, even a tiny refractive index perturbation could cause a considerable resonance shift because of the high-Q nature. The simulation results show that the circular dichroism signal is enlarged by 59 folds, and meanwhile the figure-of-merits is as large as 80.6.

Apart from the sensor applications, QBIC also provides a convenient method of designing an ultranarrow band filter by exploiting its high-Q nature. For example, a single layer of dielectric grating supports multiple symmetry-protected BICs for both TE and TM polarization. These BICs become accessible and could be selected excited by breaking the symmetry of system⁴⁰⁸⁻⁴¹¹. By applying oblique incidence, Foley et al. theoretically and experimentally realized a narrowband transmission filter in the mid-infrared wavelength range at various incident angle⁴⁰⁹. Normal incidence filtering in ultra-narrowband could be implemented by introducing the symmetry-broken for the dielectric period structure^{408,410,411}.

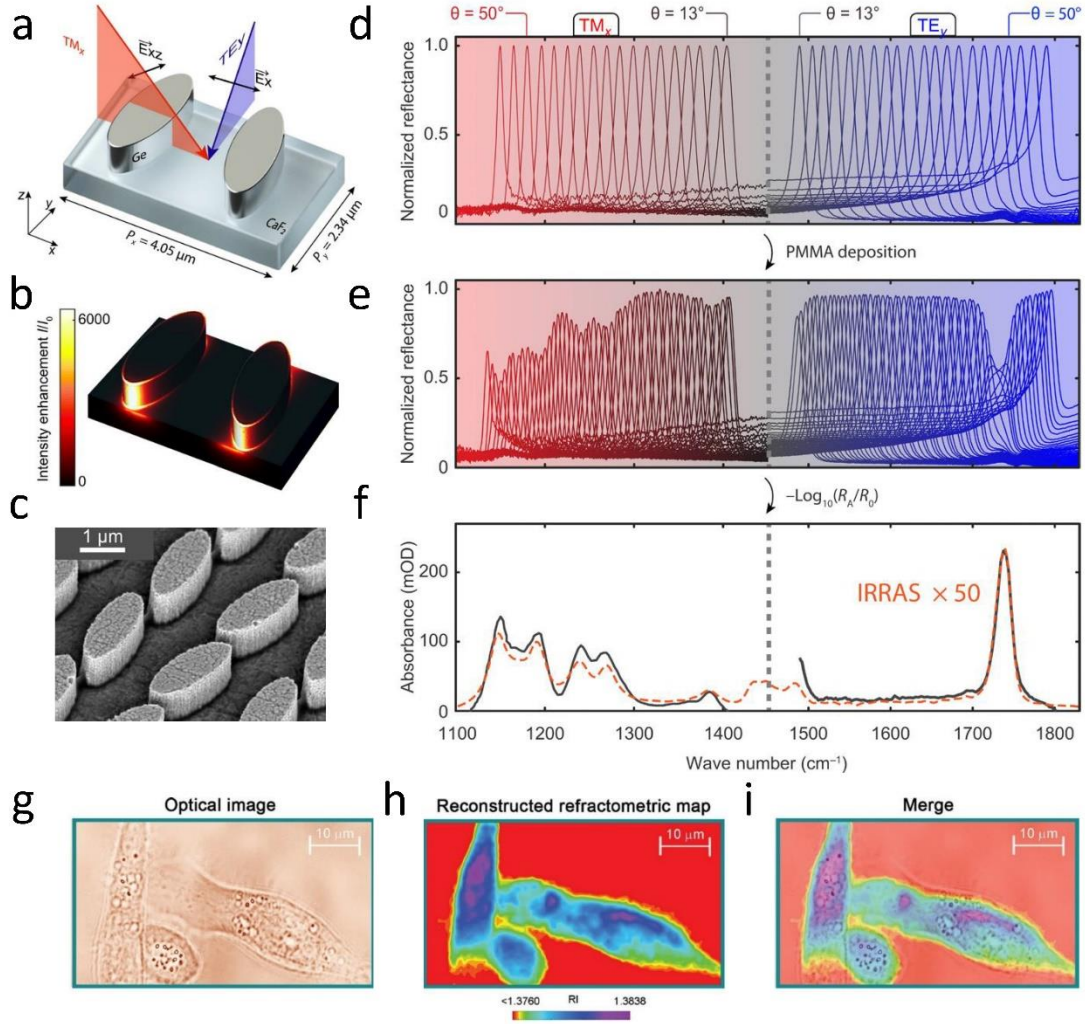


Fig.24. Biosensor based on BIC (a) Unit cell of Ge metasurface (b) Electric field distribution at QBIC. (c) SEM image of Ge metasurface. (d-e) Normalized reflection spectra before and after PMMA coating. (f) Retrieved absorbance spectrum from reflection spectra in (d) and (e). (g) optical image of prostate cancer cells PC3. (h) Reconstructed refractometric mapping from spectrum shift of quasi-BIC mode. (i) Merged image of (g) and (h). (a-f) from Ref ³⁰⁰. (g-i) from Ref ⁴⁰².

3.3.4 BIC for enhanced light absorption and strong coupling

According to the temporal coupled mode theory, light absorption contributed from a single-mode reaches a maximum value of 50% only when the critical coupling condition ($Q_{\text{rad}}=Q_{\text{abs}}$) is satisfied. Thus, the task of designing a strong light absorber turns to finding out the leaky mode with the required radiative Q-factor. QBIC is viewed as an excellent alternative to achieve this because its Q-factor can be continuously tuned by varying the structure parameters (i.e. asymmetry ratio). It is especially powerful in designing a light absorber made of low-loss materials because a high-Q mode is required to fulfill the critical coupling condition. A typical example is to boost light absorption of atomically thin two-dimensional (2D) materials, such as graphene, MoS₂, WS₂, MoSe₂ and WSe₂. By integrating such 2D materials onto an all-dielectric metasurface supporting QBIC, Xiao et al. demonstrated that the graphene absorption is enhanced to 50%⁴¹². The Q-factor of QBIC mode is tailored by shifting the hole

center inside the silicon disk array so that it can satisfy the critical coupling (Fig.25a-c). Note that such a device only works for one polarization. This restriction could be lifted by considering a metasurface whose unit cell is made of four identical Ge nanodisks⁴¹³, as demonstrated by Saadabad et al. Such a metastructure supports toroidal BICs. By introducing the nanodisk radii difference along two diagonal axes, BIC is converted into QBIC and thus the Q-factor could be continuously engineered until the critical coupling condition is satisfied. Further simulation shows that such a light absorber is polarization-independent. Moreover, if a mirror is put behind the metastructure, perfect absorption could be achieved.

Another strategy for realizing unity absorption is to find two degenerate modes that satisfy critical coupling $\omega_1=\omega_2=\omega_0$ and $Q_{\text{rad1}}=Q_{\text{rad2}}=Q_{\text{abs}}$. This strategy has been successfully applied to boost the absorption of ultrathin crystalline silicon⁴¹⁴ by Tian et al. The unit cell is an elliptical dimer, similar to the one shown in Fig.24a. Such a metastructure supports both ED-QBIC and MD-QBIC, whose Q-factors can be engineered by θ and the resonant wavelengths could be adjusted to the same value by simply changing the period along y directions. As a result, light absorption is improved to a maximum value of 84% due to the quasi-degenerate critical coupling. Note that the light absorption is not unity because both modes slightly deviate from the critical coupling. Further study may be conducted to develop advanced designs supporting degenerate BICs that simultaneously satisfy the critical coupling conditions, thus resulting in the perfect absorption.

Because BIC is viewed as a special type of cavity mode with an infinite Q-factor, it also holds great promise in realising strong coupling between excitons and photonic nanocavity. Koshelev et al. theoretically demonstrated the strong coupling by integrating WSe₂ monolayer onto Ta₂O₅ metasurface that supports BIC⁴¹⁵. Although the Q-factor is very high, The retrieved Rabi splitting from the hybrid system is only 5.7meV, slightly lower than the value 15~20 meV in dielectric metagrating system¹⁸⁶ because the electric field is localized inside the center of metastructure instead of localizing at the interface. Kravtsov et al. presented the first experimental demonstration of strong coupling between the exciton of 1L MoSe₂ and BIC mode in Ta₂O₅ grating⁴¹⁶. Because of the high-Q (Q>900) mode in metagrating, nonlinear exciton-polariton with Rabi splitting >27meV is observed. Also, the small polariton linewidth of less than 3meV enables strong polariton-polariton interaction. Later, Several other groups realize strong coupling in transition metal dichalcogenide monolayer by utilising different metastructures supporting BICs^{417,418}. Note that in above studies transition metal dichalcogenide monolayer is put on top of the periodic structure. One can further enhance the strong coupling by overlapping the field maximum and quantum emitter. Cao et al. found that by integrating WS₂ monolayer onto Si₃N₄ metagrating supporting BIC modes, the Rabi-splitting increases from 16.3meV to 28.4meV when the location of WS₂ thin film is moved from top to the position with maximum electric field⁴¹⁹. A more recent study from Al-Ani et al. shows that not only the location of WS₂ thin film but also the thickness of metagrating play essential roles in optimising the strong coupling in such a hybrid exciton-BIC system⁴²⁰ (Fig.25d-f). By considering both effects, the Rabi splitting in WS₂-SiN grating, for example, could be boosted to 65meV. In addition, the Rabi-splitting shows an increase and saturation as the Q-factor increases. This understanding may help relax the fabrication tolerance.

Another excellent alternative candidate for realizing room-temperature strong coupling is the recently emerging material-perovskite⁴²¹. It has extraordinary quantum yield and large binding energy of up to hundreds of meV. The combination of BIC and perovskite could perfectly maximize the light-matter interaction and thus form the polariton BICs. By harnessing the EPs and quasi-BICs, Lu et al. presented a theoretical study on the formation of exciton-photon polariton with perovskite metasurface on the

metallic substrate⁴²². Later, Al-Ani et al. demonstrated the optimized strong coupling in an all-perovskite metasurface⁴²³ by exploring MD-QBICs and TD-BICs. The simulated results show that the Rabi splitting in such a strongly coupled system depends not only on the Q-factor of QBIC but also on the thickness of perovskite film. The Rabi splitting could be improved to 400 meV through carefully arranging the structure parameters, representing the upper limit of strong coupling in PEPI-based perovskite metasurface. The experimental realization of polariton BIC based on PEPI perovskite metasurface has been demonstrated by two independent groups^{424,425}. The polariton BICs' nature was confirmed by angle-resolved reflection spectroscopy and PL spectroscopy, which show clear anti-crossing features. Moreover, the topological singularity inheriting from BICs was verified by measuring the Stokes parameters. Further breaking the structural symmetry of perovskite metasurface leads to a circular polarized (CP) emission. The measured degree of circular polarization (DCP) is as large as 0.835⁴²⁴. Quite recently, polariton Bose-Einstein condensation has been experimentally verified with SP-BIC supported by 1D subwavelength GaAs grating on top of GaAs multiple quantum well⁴²⁶, evidenced by a nonlinear increase of the intensity, a linewidth reduction, and a blueshift. Benefiting from BIC's infinite long lifetime and extremely near-field confinement, the threshold energy density of polariton condensation per pulse is as small as a few $\mu\text{J}/\text{cm}^2$, much lower than the counterparts of BIC-enabled laser and polariton condensation in microcavities. Besides, Such a polariton condensation inherits the topological properties from BIC by measuring the polarization vortex pattern.

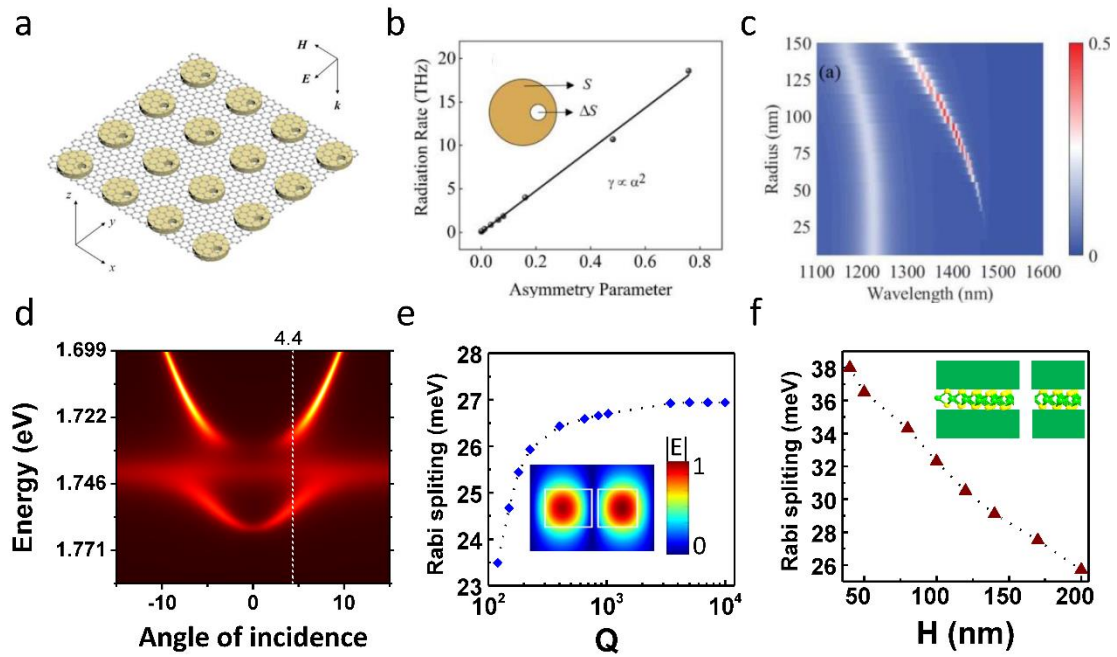


Fig.25. Enhanced light absorption and strong coupling by QBIC. (a) Schematic drawing of a graphene light absorber consisting of monolayer graphene on top of silicon metasurface supporting QBICs. (b) Radiation rate of magnetic dipole BIC vs asymmetry parameter. (c) Absorption spectra mapping as a function of the radius of off-centered hole and wavelength. (d) Absorption spectra mapping of a monolayer WSe2 on top of a SiN metagrating supporting a symmetry-protected BIC. (e) Rabi-splitting as a function of the Q-factor of QBIC. (f) Rabi splitting as a function of the height of Si₃N₄ metagrating. (a-c) from Ref ⁴¹². (d-f) from Ref ⁴²⁰.

4. PT-symmetry and EPs in photonics

In this section, we aim to review the recent progress on PT-symmetry and EPs from perspective of leaky mode engineering. Essentially speaking, the physical nature of PT-symmetry and EPs is the leaky mode engineering by tailoring the loss/gain in the coupled systems and mode coupling among them. Thus, we may view PT-symmetry and EPs as the byproduct of leaky mode engineering. However, both PT-symmetry and EPs carry the unique physical properties and lead to a diverse applications that cannot be realized with the conventional leaky modes.

4.1. PT-symmetry and EPs in photonics

Since the pioneering work of PT-symmetry by Bender et al.¹⁰⁷, different research groups have made tremendous efforts to the experimental demonstration of PT-symmetry and EPs. The first experimental realization was based on coupled passive optical waveguide by Guo et al.⁴²⁷. In this work, the loss of one waveguide is accurately controlled by a thin chromium film with different widths. As such, both EPs and phase transition were observed experimentally. In 2010, the spontaneous PT-symmetry breaking at EP was demonstrated in a coupled optical waveguide system with a balanced gain and loss⁴²⁸. Due to the broken PT-symmetry, non-reciprocal light propagation and unidirectional reflection or transmission are generated. Another excellent platform for demonstrating PT-symmetry is the coupled whisper gallery microcavity (Fig.26a-c) or coupled microring resonators, as independently demonstrated by Peng et al.⁴²⁹ and Chang et al.⁴³⁰. The non-reciprocal light transmission was observed in the nonlinear regime when PT-symmetry broken happens through carefully tailoring gain and loss and coupling strength. The nonlinearity is significantly boosted by the strong field localization of supercavity mode dominated by the gain-medium.

PT-symmetry was also realized in the periodic structure. Besides, as discussed in the first section, EPs are not just the byproduct of Hamiltonian having PT-symmetry. They also exist in the passive acoustic and photonic systems. Zhen et al. found that a lossless photonic crystal slab supports an exceptional ring⁴³¹ (Fig.26d-f), which is spawned from a Dirac cone. The dissimilar radiation decay rate of dipole and quadrupole resonance in a Dirac cone system results in the deformation of two-dimensional flat bands, finally generating a closed exceptional ring instead of an isolated EP. If the circular hole in such a photonic crystal structure is deformed into an elliptical hole, a pair of EPs are transformed into bulk Fermi arc⁴³², around which far-field radiation polarization carries a half-integer topological charge. Caselli et al. revealed that EP could also be discriminated from the generalised Fano lineshape⁴³³.

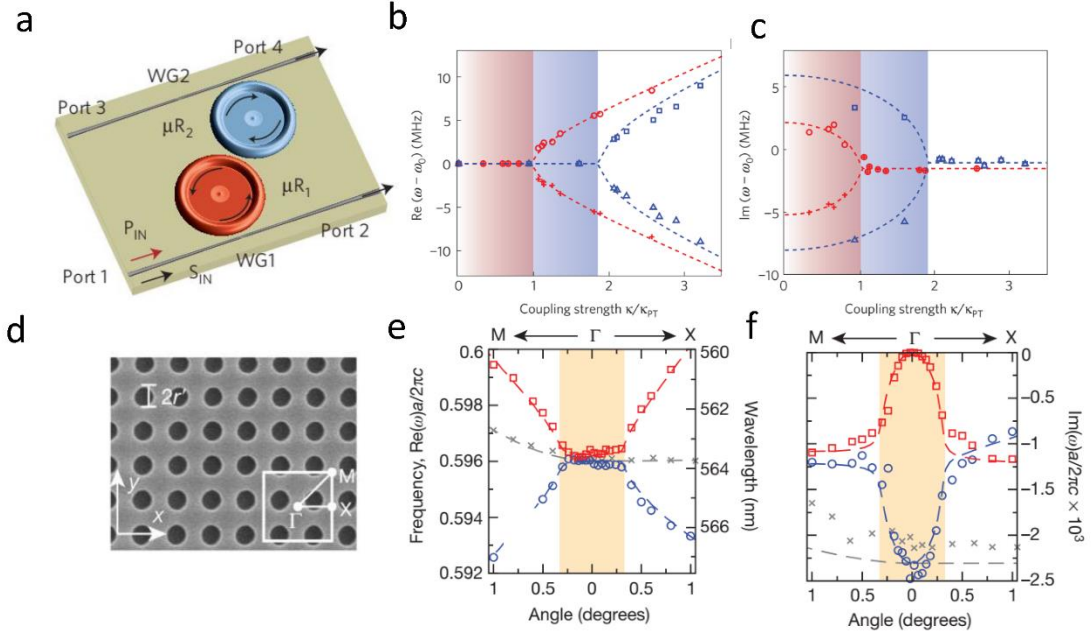


Fig.26. PT-symmetry and EP realized with different photonic platforms. (a) Schematics of coupled-microtoroid resonators system. (b-c) Real and imaginary parts of complex frequencies for coupled-resonator system vs coupling strength while μR_1 has fixed Q-factor but μR_2 has different Q-factors. (d) SEM image of fabricated photonic crystal slab that spaws exceptional ring. (e-f) Real and imaginary parts of complex eigenfrequencies retrieved from angle-resolved reflection spectroscopy. (a-c) from Ref ⁴²⁹. (d-f) from Ref ⁴³¹.

4.2 Application of PT-symmetry and EPs in photonics

4.2.1 PT-symmetry laser and EP laser

Non-Hermitian photonics have found numerous applications in developing high-performance photonics and optoelectronic devices that could not be achieved with only gain or loss medium. The most salient one among them is the single mode laser by breaking the PT-symmetry^{434,435}, as demonstrated by Feng et al. and Hodaei et al. It has been widely acknowledged that loss is detrimental to laser as it degrades the Q-factor of the system and elevates the threshold of the laser. In conventional microring cavity-based laser, lasing behavior usually happens in multimode as the high-Q whisper gallery modes are densely distributed. By introducing thresholdless PT-symmetry breaking via delicately modulating the gain and loss in the microring resonators, Feng et al. overcome the limitation of multimode lasing and realize a single mode laser⁴³⁴, as shown in Fig.27a-c. The operation principle is explained as follows: when PT-symmetry breaking happens, strong electric field localization mode sustains in the gain medium for the lasing mode, thus exhibiting net gain. In contrast, electric field is mainly distributed in the lossy medium for absorption mode. Thus, lasing happens in the former gain mode. For the rest of whisper gallery mode, the electric field is evenly distributed in the gain and loss medium, and thus PT-symmetry is maintained. The lasing frequency can be selected by carefully arranging the PT modulation on the whisper gallery mode with desired azimuthal order (Fig.27c). Meanwhile, by harnessing the PT-symmetry breaking, Hodaei et al. also demonstrated a single mode laser with coupled ring resonators⁴³⁵ (Fig.27d-f), where a balanced gain and loss is distributed in two

resonators, respectively. In 2016, Feng's group successfully demonstrated a single mode orbital angular momentum lasing by exploring the concept of EP in non-Hermitian photonics⁴³⁶.

Except for mode selection for lasing, Peng et al. found that the loss could be turned into gain when the system⁴³⁷ consisting of two coupled silica microcavities, operates within the vicinity of EP. When added loss is below the critical value, laser effect is quenched. Surprisingly, the lasing behavior was recovered for loss larger than the critical value, around which EP is formed. This finding breaks the conventional wisdom that larger loss always indicates the increasing threshold of the laser. Here, it is worth noting that although the increasing loss leads to the reduction of threshold, it is still larger than the threshold of the laser in a single silica microcavity. Later, the same group observed chiral modes and developed a unidirectional lasing⁴³⁸ in a coupled microcavities system when the system approaches EP (Fig.27g-h). Also, many other novel laser designs were proposed by taking advantage of the PT-symmetry breaking and EP.

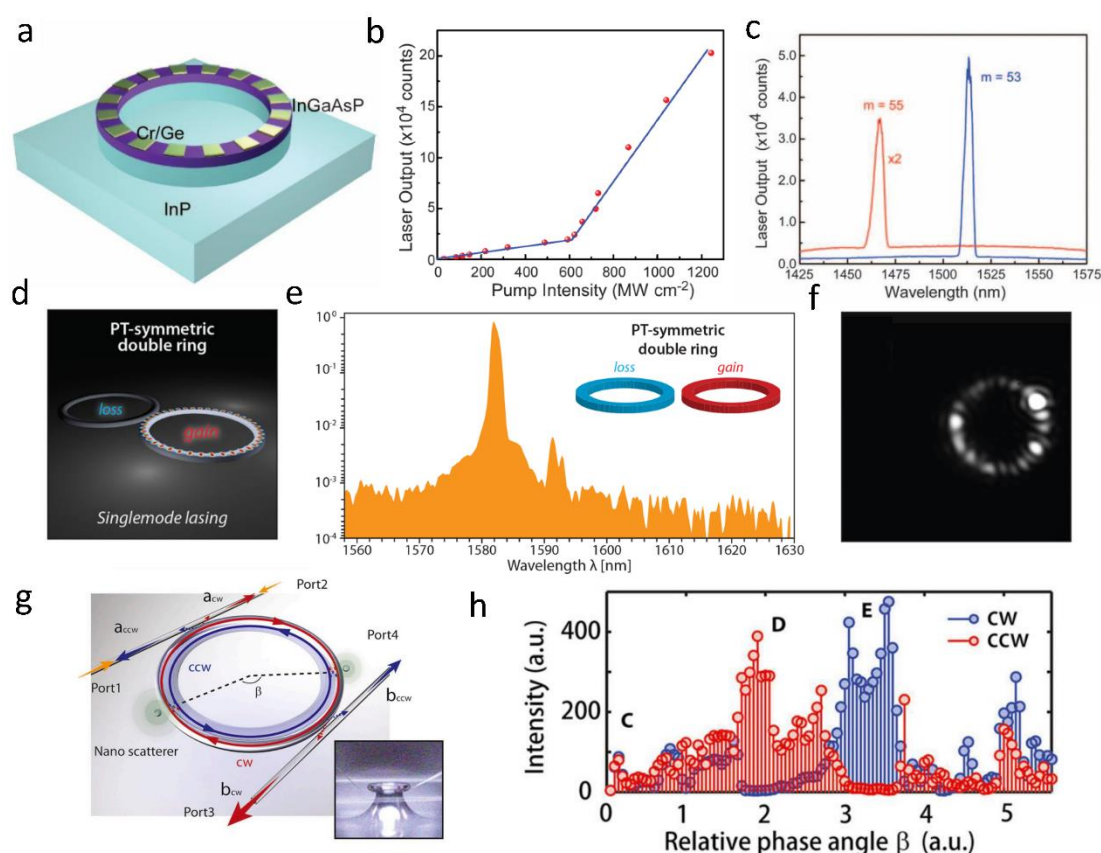


Fig.27. PT-symmetry and EP-based lasers. (a) Device configuration of PT-symmetry microring laser. (b) output emission power as a function of pump fluence. (c) Single mode laser operating at different azimuthal order. (d) Schematic drawing of microlaser based on PT symmetric double ring. (e) Single mode spectrum of PT symmetric double ring. (f) PT-symmetry broken induced lasing in the right ring. (g) Schematics of unidirectional laser based on a coupled waveguide-whisper gallery cavity. (h) Output intensity as a function of relative angle between two scatters β . (a-c) from Ref ⁴³⁴. (d-f) from Ref ⁴³⁵. (g-h) from Ref ⁴³⁸.

4.2.2 Lasing-CPA and CPA at EPs

As pointed out in Section 2.5.1, the scattering zeros and scattering poles of a lossless system are located in the first and fourth quadrants in the complex frequency plane, respectively. They are complex conjugate to each other. In other words, they share the same real part but an opposite

imaginary part. BIC corresponds to the case that both scattering zeros and scattering poles coincide at the real axis. If the gain is introduced to system, scattering poles move toward the axis of real ω . When gain increases to a critical value, one scattering pole becomes pure real, signifying the occurrence of lasing behavior. In contrast, adding loss to the system results in the downward shift of scattering zeros toward the real axis. When scattering zeros touch the real axis, a time reversal process of laser so-called coherent perfect absorption happens when a coherent light source illuminates the lossy slab from both sides¹³⁷.

Scattering zeros and poles also could coalesce at the real axis when the system satisfies the PT-symmetry. In other words, PT-symmetry scatterer could function as a laser and coherent perfect absorber^{439,440}. Taking a two-layer system satisfying PT-symmetry as an example, the gain and loss medium has a refractive index $n = n_0 \pm i\tau$ (Fig.28a). For the passive structure, scattering poles and zeros is distributed symmetrically with respect to the x axis. As shown in Fig.28b, increasing τ drives the poles and zeros first move along horizontal directions, and then move along vertical axis. These two processes represent the PT-symmetry phase and PT-symmetry breaking phase, which are connected by the phase boundary or the transition point. The first experimental demonstration on lasing and CPA with a single cavity was done by Wong et al. in 2016⁴⁴¹. In this work, the authors utilized a waveguide structure with gain-loss PT modulation, in which the InGaAsP multiple quantum well serves as gain medium and periodic Cr/Ge strips distributed on top introduce loss to the system (Fig.28c). By carefully tuning the frequency, amplitude and phase of illumination beams, CPA-laser was observed in the same optical devices (Fig.28d). The lasing-antilasing behavior was confirmed by checking the extinction ratio, which is defined as the ratio of two output intensities to two input intensities. Measurement results showed that the extinction ratio increases from -20 dB (CPA or antilasing state) to 15dB (lasing state) by simply changing the phase offset between two probe beams from $\frac{\pi}{2}$ to $-\frac{\pi}{2}$.

Generally speaking, EPs could be accessed in either a lossless structure (i.e. photonic crystal slab), lossy structure or PT-symmetry system with balanced gain and loss. This kind of EP has been termed as resonant EPs. A recent study further extended the concept of EP to the degenerate scattering zeros so called absorption EP⁴⁴². CPA EP is a special case of absorption EP. It is formed only when two scattering zeros coalesce at the real axis. The key difference between CPA and CPA EP lies in the fact that absorption line shape is quadratic for the former while the latter has a quartic line shape (Fig.28e). This interesting property has been demonstrated experimentally by two independent groups. In Ref ⁴⁴³, Wang et al. deliberately designed a coupled microtoroid system, which is coupled in and out via one or two fiber waveguides. Generic CPA EP was found in one channel system by adjusting both the coupling between waveguide and microcavity (Fig.28f). This phenomenon is equivalent to the critical coupling at EP. Also, non-generic CPA EP has been implemented in a two-channel system by properly choosing the phase difference between two coherence sources (Fig.28g). In fact, the restriction of realising non-generic CPA is less rigorous than that of generic CPA because resonant EP also happens, and thus it may be much easier to realize non-generic CPA than generic CPA. In Ref ⁴⁴⁴, Soleymani et al. leverage an exceptional surface in a waveguide-coupled resonator system to achieve perfect chiral absorption at critical coupling conditions. It is also interesting that super-absorption could be achieved even in dielectric metasurfaces by breaking the PT-symmetry⁴⁴⁵. In this case, EP degeneracies with two nonorthogonal QBICs are made to enable perfect absorption.

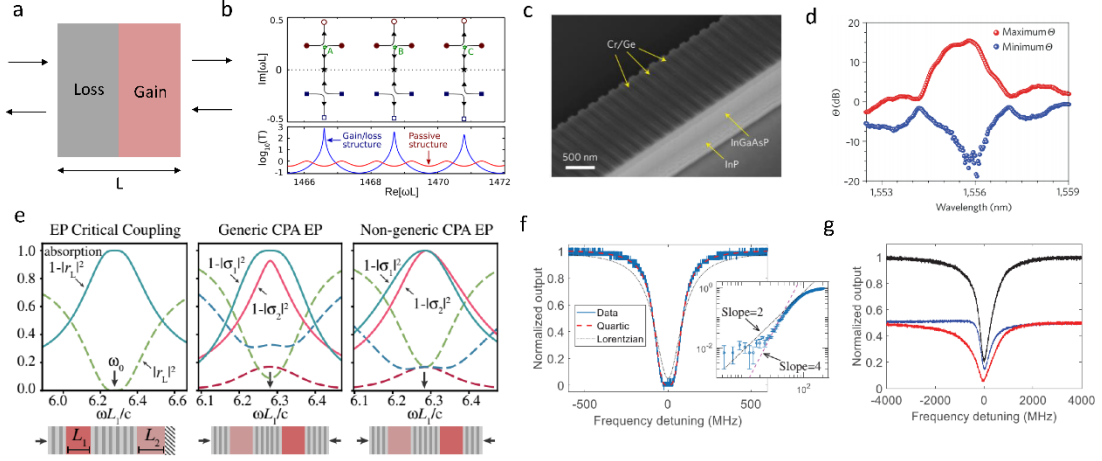


Fig.28. (a) Schematics of a two-layers PT-symmetric system ($n = n_0 \pm i\tau$). (b) The top panel shows the evolution of scattering zero and poles when imaginary part of the refractive index τ is increased. The bottom panel is transmittance spectrum for the passive system ($\tau=0$) and PT-symmetric system ($\tau=0.05$). (c) SEM image of laser and CPA. (d) Spectrum output spectrum of the device operating at CPA mode and laser mode. (e) The top panel shows absorption and reflection spectrum at CPA EP when the cavity is truncated by asymmetric and symmetric mirror. The bottom panel shows the cavity structure with asymmetric and symmetric mirrors. (f) Measured normalized output at CPA EP for a single port system. (g) Measured normalized output at nongeneric CPA EP. (a-b) from Ref ⁴⁴⁰. (c-d) from Ref ⁴⁴¹. (e) from Ref ⁴⁴². (f-g) from Ref ⁴⁴³.

4.2.3 EP sensor

One of the prominent applications of EP is sensors. Unlike the BIC-based optical sensor that measures the resonant wavelength shift when external environment perturbation is introduced, EP or diabolic point-based sensor's performance is characterized by the frequency split^{446,447}. The diabolic point has degenerate eigen-energy levels (degeneracy ≥ 2) but no degenerate eigenstates. The corresponding eigenstates are chosen to be orthogonal to each other. However, both energy levels and eigenstates are degenerate for EPs. Typically, diabolic points rely on mode degeneracy, which can be easily realized by whispery gallery modes in microdisk and microrings. For ultrasmall perturbation ϵ , the sensitivity at N-order EP is proportional to $\epsilon^{1/N}$, higher than the sensitivity based on diabolic point which is proportional to ϵ . A simple proof is presented for a two-level system with degenerate eigenvalues⁴⁴⁷. For conventional degeneracy diabolic point, its Hamiltonian could be represented by a 2×2 matrix,

$$H_{DP} = \begin{pmatrix} E_0 & 0 \\ 0 & E_0 \end{pmatrix} \quad (31)$$

where E_0 is the complex eigenvalue.

For the case of EP, its Hamiltonian could not be diagonalized and thus has the following form,

$$H_{EP} = \begin{pmatrix} E_0 & A_0 \\ 0 & E_0 \end{pmatrix} \quad (32)$$

where both E_0 and A_0 are complex.

Defining the non-hermitian Hamiltonian as

$$H_1 = \begin{pmatrix} E_1 & A_1 \\ B_1 & E_1 \end{pmatrix} \quad (33)$$

Adding a non-hermitian Hamiltonian perturbation ϵH_1 to Hamiltonian of DP and EP and solving the new Hamiltonian gives the eigenvalue splits as follows

$$\Delta E_{DP} = 2\epsilon\sqrt{A_1B_1} \quad (34a)$$

$$\Delta E_{EP} = 2\sqrt{\epsilon}\sqrt{A_0B_1 + \epsilon A_1B_1} \quad (34b)$$

For very tiny perturbations ($\epsilon \ll 1$ or $|A_0| \gg |A_1|$), the eigenvalue split for EP is proportional to $\sqrt{\epsilon}$, much larger than the eigenvalue split of DP proportional to ϵ . The enhanced ratio is expressed as

$$\frac{\Delta E_{EP}}{\Delta E_{DP}} = \frac{\sqrt{A_0/A_1 + \epsilon}}{\sqrt{\epsilon}} \quad (35)$$

The excellent sensitivity of EP compared to DP was experimentally demonstrated by two research groups in 2017^{448,449}. Chen et al. adopt the coupled silica microcavities coupled to a fibre-taper waveguide⁴⁴⁸. Two nano-tips are introduced to bring the system to EP. Then, the third silica nano-tip scatter serving as perturbation is brought close to the system to characterize the performance of EP-based sensors. For the conventional DP-based NP sensors, only one silica nano-tip is required to remove the degeneracy of counter-clockwise and clock-wise whisper gallery mode. From Fig.29a-b, the frequency splits for EP and DP sensors are indeed proportional to $\sqrt{\epsilon}$ and ϵ , respectively. It is worth pointing out that after passing through EP, the linewidths of two resonances become broadened if only scattering loss is introduced. This may reduce the spectrum resolvability and limit the EP sensor's performance. This obstacle has been removed by using a balanced gain-loss system. Another parallel work by Hodaie et al. realized second and third-order EP sensors through coupled ring resonators system⁴⁴⁹(Fig.29c-d), in which gain and loss could be independently controlled in each resonator. Experimental measurement verified that the frequency splits of second and third-order EP follow square root and cube root law. In 2019, EP was utilized to enhance the sensitivity of the optical gyroscope by amplifying the Sagnac effect^{450,451}. Although the EP sensor has shown superior performance than the conventional DP sensor, there are still some challenges before it is used for commercial applications. As an EP is usually enabled via delicate control on loss or coupling strength between resonators, every detection will make the system deviate from EP. One has to bring the system back to EP after each detection, which may not be an easy task. Otherwise, the EP sensor's performance will degrade with the use time. To make the system robust against unwanted perturbation, Zhong et al. proposed an exceptional surface sensor showing enhanced sensitivity and robustness⁴⁵².

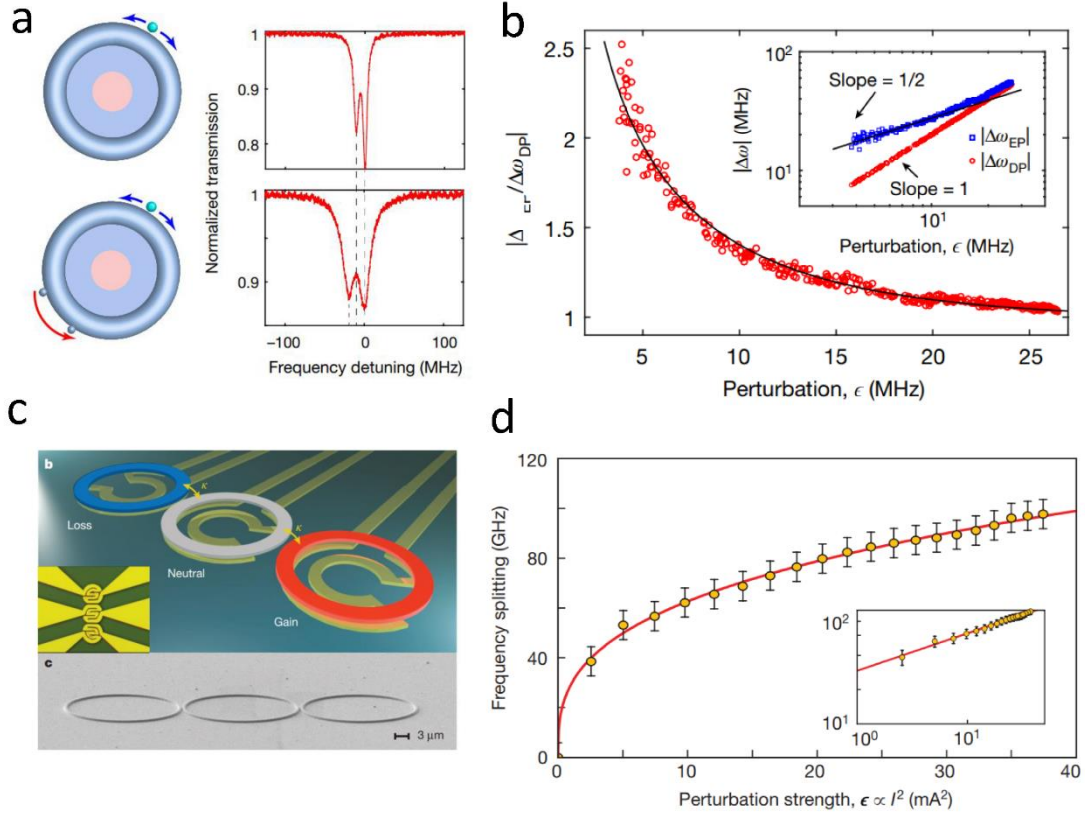


Fig.29. EP sensor (a) transmission spectra of a diabolic sensor and EP sensor. (b) Frequency splitting enhancement factor as a function of perturbation. (c) Schematic drawing of three-order EP sensor consisting of PT symmetric coupled micro-ring resonator system. (b) SEM image of fabricated coupled micro-ring resonator system. (c-d) Frequency splitting as a function of perturbation. (a-b) from Ref ⁴⁴⁸. (c-d) from Ref ⁴⁴⁹.

5. Conclusion and outlook

Leaky modes are the eigenmodes of an open non-Hermitian system. Their properties depend only on the material and shape of the structure and the environments in which the structures are embedded. Leaky modes supported by all-dielectric metasystems have demonstrated their powerful ability to govern their optical properties and enhance light-matter interactions. Thus, we present a comprehensive review of recent progress of the all-dielectric metasystem from leaky modes perspective, highlighting the fundamental physics behind leaky modes and their applications in boosting light-matter interaction. Although giant progress has been made in these topics, there are still many opportunities awaiting exploration.

- (a) In section 2, many interesting physics phenomena, such as antireflection coating, superscattering and perfect absorber, have been predicted and interpreted with temporal coupled mode theory. However, how to find leaky modes required for fulfilling these exotic phenomena step by step remains an open question. For example, it has been proved that degenerate modes satisfying critical coupling could lead to perfect absorption. How to construct degenerate modes that achieve critical coupling is still not resolved. Also, leaky modes have been revealed to be linked to polarization states for a photonic crystal slab sitting on the perfect electric conductor substrate. It might be interesting to generalize this to the dielectric metasystem without and with substrate

because it will empower the leaky modes to construct any polarization states. Leaky modes' applications are much broader and are far beyond what we have discussed. For instance, leaky modes have found great success in radiative cooling⁴⁵³⁻⁴⁵⁵. Also, they have been used for realizing mathematic operation and image differentiation⁴⁵⁶⁻⁴⁶². Additionally, the role of leaky modes supported by Huygen's metasurface has been clarified in controlling the wavefront of electromagnetic wave^{463,464}. More research shall be conducted to optimize these photonic devices with superior performance. Besides, it is well documented that the mode volume of leaky modes in dielectric resonators is usually much larger than the mode volume of plasmonic resonators. This is because the electric field distributes inside and around the dielectric resonators while the electric field is mainly localized at the interface of metallic nanostructures. However, the Q-factor of leaky modes is much larger than the counterpart of plasmonic resonator. Increasing attention has been paid to studying the hybrid dielectric-metallic resonator⁴⁶⁵⁻⁴⁶⁹ because it captures both the advantages of dielectric resonators and plasmonic resonators. In real applications like laser or strong coupling, large Q-factor and ultrasmall mode volume are desired⁴⁷⁰. A hybrid dielectric-metallic system may provide a perfect solution for this.

- (b) Bound states in the continuum have witnessed massive progress in the past ten years, ranging from fundamental physics to practical applications. There are also some questions remaining unanswered. For symmetry-broken induced QBICs, their Q-factors are inversely proportional to α^{-2} (α is the asymmetry parameter). However, in real fabrication, it is very challenging to achieve an ultrasmall α to obtain an ultrahigh Q-factor. Currently, most of the Q-factor of symmetry-broken induced QBICs reported experimentally is 50~5000, far away from the high-Q factor enabled by microring/microdisk resonators. Thus, it is necessary to develop a general recipe that could accurately control the asymmetry parameters. Moreover, the substrate has been regarded as a detrimental factor that reduces the Q-factor of QBIC because it introduces additional leaky channels. How to alleviate the substrate effect is also an open question. Additionally, topological BICs have been reported in the momentum space due to the merged topological charge of multiple BICs. It may bring more fabrication tolerance if merged BICs could be constructed in geometry parameter space^{471,472}. Besides, the correlation between QBICs in a single dielectric NP and BICs in an array of dielectric structures has not been revealed. Besides, most of the BICs reported so far are low-order multipolar BICs, such as magnetic dipole BIC and toroidal dipole BICs. We may expect more research on exploring high-order multipolar BICs as they could bring more freedom in tailoring the far-field scattering. Last but not least, although QBICs have been found in a single dielectric NP, their Q-factors are still moderate. One may expect an increased Q-factor via engineering the coupling between NPs if several dielectric NPs are placed together. On the application side, there is a bright future for BICs because they could be integrated with novel nanomaterials and quantum emitters, such as two-dimensional materials and perovskite. Also, dynamic tuning BICs with phase change materials has not been explored.
- (c) PT-symmetry and EPs provide a new way of manipulating the electromagnetic wave by tailoring gain and loss in coupled resonators. Similar to the case of BICs, EPs also carry topological charges in far-field radiation. However, the topological charge of EPs is associated with a nontrivial Chern number while BICs is associated with polarization singularities. Thus, it is necessary to reveal whether these two are connected or not. Also, in section II, a simple two-level system predicted that tuning the complex coupling could switch BICs to EPs. Some efforts have been made to build BICs and EPs in the same photonic platform⁴⁷³. It is interesting to see whether it is possible to tune

the system from BICs to EPs dynamically.

Appendix.A-Leaky Modes in a single dielectric structure

We first derive the eigenvalues of leaky modes supported by single dielectric nanostructures, including 1D slab, 2D cylinder and 3D particle. We tackle this problem in two different ways: boundary-matching conditions and scattering poles.

(1) Boundary Matching condition

Case 1: 1D Fabry Perot slab with a refractive index as n_2 embedded into background medium with a refractive index as n_1

Note $\exp(-i\omega t)$ is assumed during the following derivation process

Assume E_x-H_y and interface located at $z=-L/2$ and $z=L/2$

Solving the Maxwell equations, one can have the electric field as follows

$$E_x(z)=A \exp(+in_1k_0z), \quad z>L/2 \quad (A1a)$$

$$E_x(z)=B.\exp(-in_2k_0z)+C.\exp(+in_2k_0z), \quad -L/2<z<L/2 \quad (A1b)$$

$$E_x(z)=D \exp(-in_1k_0z), \quad z<-L/2 \quad (A1c)$$

Also, the magnetic field H can be obtained by following equations

$$i\omega\mu_0 H_y = \frac{\partial E_x}{\partial z} \quad (A2)$$

Substituting Eq.(A1) into Eq.(A2), we will have

$$H_y(z)=A.(n_1\mu_0/c). \exp(+in_1k_0z), \quad z>L/2 \quad (A3a)$$

$$H_y(z)=B.(-n_2\mu_0/c).\exp(-in_2k_0z)+C. (n_2\mu_0/c).\exp(+in_2k_0z), \quad -L/2<z<L/2 \quad (A3b)$$

$$H_y(z)=D.(-n_1\mu_0/c). \exp(-in_1k_0z), \quad z>L/2 \quad (A3c)$$

By matching the continuity of boundary conditions at $z=-L/2$ and $z=L/2$,

$$A \exp(in_1k_0L/2)= B.\exp(-in_2k_0L/2)+C.\exp(+in_2k_0L/2) \quad (A4a)$$

$$D \exp(in_1k_0L/2)= B.\exp(+in_2k_0L/2)+C.\exp(-in_2k_0L/2) \quad (A4b)$$

$$A.(n_1)\exp(in_1k_0L/2)= B.(-n_2).\exp(-in_2k_0L/2)+C.n_2.\exp(+in_2k_0L/2) \quad (A4c)$$

$$D.(-n_1)\exp(in_1k_0L/2)= B.(-n_2).\exp(+in_2k_0L/2)+C.n_2.\exp(-in_2k_0L/2) \quad (A4d)$$

$$(A4a)*n_1-(A4c): (n_1+n_2).\exp(-in_2k_0L/2).B+(n_1-n_2). \exp(+in_2k_0L/2).C=0 \quad (A5a)$$

$$(A4b)*n_1+(A4c): (n_1-n_2).\exp(+in_2k_0L/2).B+(n_1+n_2). \exp(-in_2k_0L/2).C=0 \quad (A5b)$$

Or

$$(n_1+n_2).\exp(-in_2k_0L/2).B=(n_2-n_1). \exp(+in_2k_0L/2).C \quad (A6a)$$

$$(n_2-n_1).\exp(+in_2k_0L/2).B=(n_1+n_2). \exp(-in_2k_0L/2).C \quad (A6b)$$

$$(6a)*(6b): B^2=C^2, \text{ or } B= \pm C \quad (A7)$$

Substituting eq.(A7) into eq.(A5a), we will have

$$(n_1+n_2)/(n_2-n_1)= \pm \exp(in_2k_0L) \quad (A8)$$

Eq.(A8) is the same as Eq.(2.4) in ref ¹⁷, where +/- indicates even/odd modes.

Regarding the coefficients A, B, C, D, they are determined by the normalization.

Lasing behavior: Introducing gain material is equivalent to adding a negative imaginary part into the refractive index. We illustrate this example in the following

Considering $n_2=4-bi$, $n_1=1$. $(5-bi)/(3-bi)=+\exp(i*(4-bi)*k_0L)$.

In order to make k_0L is real, one will have

$(25+b^2)/(9+b^2)=\exp(2b^2*k_0L)$, assume $b=0.1$, one will have lasing mode at $(25+0.01)/(9+0.01)=\exp(0.02*k_0L)$

Case 2: 2D dielectric cylinder ($n=n_2$) embedded into background ($n=n_1$)

TE (E//z): cylindrical coordinates (r, ϕ, z)

$$E_z(r, \phi, z) = C \frac{J_m(\kappa r)}{J_m(\kappa r_0)} e^{i\beta z} e^{im\phi}, \quad r \leq r_0 \quad (A9a)$$

$$E_z(r, \phi, z) = C \frac{H_m(\gamma r)}{H_m(\gamma r_0)} e^{i\beta z} e^{im\phi}, \quad r > r_0 \quad (A9b)$$

Where $\kappa^2 = n_2^2 k^2 - \beta^2$ and $\gamma^2 = n_1^2 k^2 - \beta^2$

Since we are interested in plane propagation, β should be set as $\beta=0$. Otherwise, it may be treated as waveguide modes.

Then, Eq.(A9) can be rewritten as

$$E_z(r, \phi, z) = C \frac{J_m(n_2 \kappa r)}{J_m(n_2 \kappa r_0)} e^{im\phi}, \quad r \leq r_0 \quad (A9a)$$

$$E_z(r, \phi, z) = C \frac{H_m(n_1 \kappa r)}{H_m(n_1 \kappa r_0)} e^{im\phi}, \quad r > r_0 \quad (A9b)$$

The transverse component of H_ϕ can be obtained as follows

$$H_\phi(r, \phi, z) = -\frac{i\omega\epsilon_2}{\epsilon_2 k^2} \frac{\partial E_z}{\partial r} = -\frac{ic}{k} \frac{\partial E_z}{\partial r}, \quad r \leq r_0 \quad (A10a)$$

$$H_\phi(r, \phi, z) = -\frac{i\omega\epsilon_1}{\epsilon_1 k^2} \frac{\partial E_z}{\partial r} = -\frac{ic}{k} \frac{\partial E_z}{\partial r}, \quad r > r_0 \quad (A10b)$$

Matching the boundary condition gives us

$$n_2 \frac{J'_m(n_2 \kappa r_0)}{J_m(n_2 \kappa r_0)} = n_1 \frac{H'_m(n_1 \kappa r_0)}{H_m(n_1 \kappa r_0)}, \quad \text{TE} \quad (A11)$$

TM(H//z): cylindrical coordinates (r, ϕ, z)

$$H_z(r, \phi, z) = D \frac{J_m(\kappa r)}{J_m(\kappa r_0)} e^{i\beta z} e^{im\phi}, \quad r \leq r_0 \quad (A12a)$$

$$H_z(r, \phi, z) = D \frac{H_m(\gamma r)}{H_m(\gamma r_0)} e^{i\beta z} e^{im\phi}, \quad r > r_0 \quad (A12b)$$

Where $\kappa^2 = n_2^2 k^2 - \beta^2$ and $\gamma^2 = n_1^2 k^2 - \beta^2$

Similarly, in plane propagation indicates $\beta=0$.

Then, Eq.(A12) can be rewritten as

$$H_z(r, \phi, z) = D \frac{J_m(n_2 \kappa r)}{J_m(n_2 \kappa r_0)} e^{im\phi}, \quad r \leq r_0 \quad (A13a)$$

$$H_z(r, \phi, z) = D \frac{H_m(n_1 \kappa r)}{H_m(n_1 \kappa r_0)} e^{im\phi}, \quad r > r_0 \quad (A13b)$$

The transverse component of E_ϕ can be obtained as follows

$$E_\phi(r, \phi, z) = \frac{i\omega\mu_2}{\epsilon_2 k^2} \frac{\partial H_z}{\partial r} = \frac{ic}{n_2^2 k} \frac{\partial H_z}{\partial r}, \quad r \leq r_0 \quad (A14a)$$

$$E_\phi(r, \phi, z) = \frac{i\omega\mu_1}{\varepsilon_1 k^2} \frac{\partial H_z}{\partial r} = \frac{ic}{n_1^2 k} \frac{\partial H_z}{\partial r}, \quad r > r_0 \quad (\text{A14b})$$

Matching the boundary condition gives us

$$\frac{J'_m(n_2 k r_0)}{n_2 J_m(n_2 k r_0)} = \frac{H'_m(n_1 k r_0)}{n_1 H_m(n_1 k r_0)} \quad (\text{A15})$$

Case 3: 3d dielectric sphere (n=n₂) embedded into background (n=n₁)

For TE polarization (E_r=0)

$$E_t(r, \phi, z) = C \cdot j_n(n_2 k r) \cdot F(\theta, \phi), \quad r \leq r_0 \quad (\text{A16a})$$

$$E_t(r, \phi, z) = C' \cdot h_n(n_1 k r) \cdot F(\theta, \phi), \quad r > r_0 \quad (\text{A16a})$$

From Maxwell equation $H = \frac{(\nabla \times E)}{i\omega\mu}$

We will have magnetic field as

$$H_t(r, \phi, z) = C \cdot \frac{n_2 k}{i\omega\mu} \frac{[n_2 k r \cdot j_n(n_2 k r)]'}{n_2 k r} \cdot G(\theta, \phi), \quad r \leq r_0 \quad (\text{A17a})$$

$$H_t(r, \phi, z) = C' \cdot \frac{n_1 k}{i\omega\mu} \frac{[n_1 k r \cdot h_n(n_1 k r)]'}{n_1 k r} \cdot G(\theta, \phi), \quad r > r_0 \quad (\text{A17a})$$

Matching the boundary condition at $r=r_0$ will give us

$$C \cdot j_n(n_2 k r_0) \cdot F(\theta, \phi) = C' \cdot h_n(n_1 k r_0) \cdot F(\theta, \phi) \quad (\text{A18a})$$

$$C \cdot \frac{n_2 k}{i\omega\mu} \frac{[n_2 k r \cdot j_n(n_2 k r)]'_{r=r_0}}{n_2 k r_0} \cdot G(\theta, \phi) = C' \cdot \frac{n_1 k}{i\omega\mu} \frac{[n_1 k r \cdot h_n(n_1 k r)]'_{r=r_0}}{n_1 k r_0} \cdot G(\theta, \phi) \quad (\text{A18b})$$

(A18b)/(A18a) will give us

$$\frac{[n_2 k r \cdot j_n(n_2 k r)]'_{r=r_0}}{j_n(n_2 k r_0)} = \frac{[n_1 k r \cdot h_n(n_1 k r)]'_{r=r_0}}{h_n(n_1 k r_0)} \quad (\text{A19})$$

Similarly, for TM polarization (H_r=0)

$$H_t(r, \phi, z) = D \cdot j_n(n_2 k r) \cdot F(\theta, \phi), \quad r \leq r_0 \quad (\text{A20a})$$

$$H_t(r, \phi, z) = D' \cdot h_n(n_1 k r) \cdot F(\theta, \phi), \quad r > r_0 \quad (\text{A20a})$$

From Maxwell equation $E = -\frac{(\nabla \times H)}{i\omega\varepsilon}$

We will have electric fields as

$$E_t(r, \phi, z) = -D \cdot \frac{n_2 k}{i\omega n_2^2} \frac{[n_2 k r \cdot j_n(n_2 k r)]'}{n_2 k r} \cdot G(\theta, \phi), \quad r \leq r_0 \quad (\text{A21a})$$

$$E_t(r, \phi, z) = -D' \cdot \frac{n_1 k}{i\omega n_1^2} \frac{[n_1 k r \cdot h_n(n_1 k r)]'}{n_1 k r} \cdot G(\theta, \phi), \quad r > r_0 \quad (\text{A21a})$$

Matching boundary condition at $r=r_0$ gives us

$$D \cdot j_n(n_2 k r_0) \cdot F(\theta, \phi) = D' \cdot h_n(n_1 k r_0) \cdot F(\theta, \phi) \quad (\text{A22a})$$

$$D \cdot \frac{n_2 k}{i\omega n_2^2} \frac{[n_2 k r \cdot j_n(n_2 k r)]'_{r=r_0}}{n_2 k r_0} \cdot G(\theta, \phi) = D' \cdot \frac{n_1 k}{i\omega n_1^2} \frac{[n_1 k r \cdot h_n(n_1 k r)]'_{r=r_0}}{n_1 k r_0} \cdot G(\theta, \phi) \quad (\text{A22b})$$

(A22b)/(A22a) will give us

$$\frac{[n_2 k r \cdot j_n(n_2 k r)]'_{r=r_0}}{n_2^2 j_n(n_2 k r_0)} = \frac{[n_1 k r \cdot h_n(n_1 k r)]'_{r=r_0}}{n_1^2 h_n(n_1 k r_0)} \quad (\text{A23})$$

(2) Poles of the scattering matrix

Case 1: 1D Fabry Perot slab with a refractive index as n_2 embedded into the background with a refractive index as n_1

Assume normal incidence, we will have

$$E_r = E_0 r + E_0 t t' r' e^{i\delta} + E_0 t t' r'^3 e^{i2\delta} + E_0 t t' r'^5 e^{i3\delta} + \dots \quad (A24)$$

$$E_r = E_0 r + E_0 t t' r' e^{i\delta} (1 + r'^2 e^{i\delta} + r'^4 e^{i2\delta} + \dots) \quad (A25)$$

$$E_r = E_0 r + E_0 t t' r' \frac{e^{i\delta}}{1 - r'^2 e^{i\delta}} \quad (A26)$$

Then reflection can be obtained by

$$R = \frac{I_r}{I_0} = \frac{|E_r|^2}{|E_0|^2} = \left| r + \frac{t t' r' e^{i\delta}}{1 - r'^2 e^{i\delta}} \right|^2 \quad (A27)$$

Where $r = (n_1 - n_2)/(n_1 + n_2)$, $r' = -r$, $t = 1 + r$, $t' = 1 + r'$, $\delta = 2n_2 k d$

$$R = \frac{I_r}{I_0} = \frac{4r^2 \sin^2(\frac{\delta}{2})}{(1 - r^2)^2 + 4r^2 \sin^2(\frac{\delta}{2})} \quad (A28)$$

Checking the scattering poles gives us

$$(1 - r^2)^2 + 4r^2 \sin^2(\frac{\delta}{2}) = 0 \quad (A29)$$

After some mathematical manipulation, one will have

$$(1 - r^2 e^{i\delta})(1 - r^2 e^{-i\delta}) = 0 \quad (A30)$$

Only the first term=0 is the poles of the scattering matrix

$$(1 - r^2 e^{i\delta}) = 0 \quad (A31)$$

Note that from Eq.(A27), one can immediately find the poles of scattering matrix.

This is exactly the same as the one derived above and the results in paper of LPR.

More about scattering matrix

$$r_{12} = r_{21} = r - \frac{(1 - r^2) r e^{i\delta}}{1 - r^2 e^{i\delta}} \quad (A32)$$

For transmission

$$E_t = E_0 t t' e^{\frac{i\delta}{2}} + E_0 t t' r'^2 e^{\frac{i3\delta}{2}} + E_0 t t' r'^4 e^{\frac{i5\delta}{2}} + E_0 t t' r'^6 e^{\frac{i7\delta}{2}} + \dots \quad (A33a)$$

$$E_t = E_0 t t' e^{\frac{i\delta}{2}} (1 + r'^2 e^{i\delta} + r'^4 e^{i2\delta} + r'^6 e^{i3\delta} + \dots) \quad (A33b)$$

$$t_{12} = t_{21} = \frac{t t' e^{i\delta/2}}{1 - r'^2 e^{i\delta}} = \frac{(1 - r^2) e^{i\delta/2}}{1 - r^2 e^{i\delta}} \quad (A34)$$

Eigenvalue of Scattering matrix

$$d = r_{12} \pm t_{12} \quad (A35)$$

if $d=0$, then $(1 - r^2) e^{i\delta/2} \pm r(1 - e^{i\delta}) = 0$. Solving this equation gives us $e^{i\delta/2} = \pm r$

Case 2: 2D dielectric cylinder ($n=n_2$) embedded into background ($n=n_1$)

For an isolated dielectric cylinder, its scattering cross-section can be evaluated by

$$Q_{scs}^{p,s} = \frac{4}{k} \sum_{m=-\infty}^{\infty} |a_m^{p,s}|^2 \quad (A36)$$

p polarization—H/z (TM)

$$a_m^p = a_{-m}^p = \frac{n_2 J_m(n_2 k r) J'_m(n_1 k r) - n_1 J_m(n_1 k r) J'_m(n_2 k r)}{n_2 J_m(n_2 k r) H'_m(n_1 k r) - n_1 H_m(n_1 k r) J'_m(n_2 k r)} \quad (A37a)$$

s polarization---E//z (TE)

$$a_m^s = a_{-m}^s = \frac{n_2 J_m(n_1 kr) J_m'(n_2 kr) - n_1 J_m(n_2 kr) J_m'(n_1 kr)}{n_2 H_m(n_1 kr) J_m'(n_2 kr) - n_1 J_m(n_2 kr) H_m'(n_1 kr)} \quad (A37b)$$

By checking the poles of scattering efficiency, one will have

$$n_2 J_m(n_2 kr) H_m'(n_1 kr) = n_1 H_m(n_1 kr) J_m'(n_2 kr), \text{ TM} \quad (A38a)$$

$$n_2 H_m(n_1 kr) J_m'(n_2 kr) = n_1 J_m(n_2 kr) H_m'(n_1 kr), \text{ TE} \quad (A38b)$$

Comparing Eq.(A38) with Eq. (A11) and Eq.(A15), we will find they are the same.

Case 3: 3d dielectric sphere (n=n₂) embedded into background (n=n₁)

For an isolated dielectric sphere, its scattering cross-section can be evaluated by

$$Q_{scs} = \frac{2\pi}{k^2} \sum_{n=1}^{\infty} (2n+1) (|a_n|^2 + |b_n|^2) \quad (A39)$$

a_n and b_n are scattering efficiency, and can be expressed as follows

$$a_n = \frac{m^2 j_n(mx) [x j_n(x)]' - j_n(x) [mx j_n(mx)]'}{m^2 j_n(mx) [x h_n^{(1)}(x)]' - h_n^{(1)}(x) [mx j_n(mx)]'} \quad (A40a)$$

$$b_n = \frac{j_n(mx) [x j_n(x)]' - j_n(x) [mx j_n(mx)]'}{j_n(mx) [x h_n^{(1)}(x)]' - h_n^{(1)}(x) [mx j_n(mx)]'} \quad (A40b)$$

where m=n₂/n₁, x=n₁kr₀

Checking the poles of scattering efficiency (denominator=0) will give us

$$m^2 j_n(mx) [x h_n^{(1)}(x)]' = h_n^{(1)}(x) [mx j_n(mx)]' \quad (A41a)$$

$$j_n(mx) [x h_n^{(1)}(x)]' = h_n^{(1)}(x) [mx j_n(mx)]' \quad (A41b)$$

Comparing Eq. (A41) with Eq. (A19) and Eq.(A23), we will find that they are the same.

Appendix-B-Proof that Hamiltonian in Eq. (21) is PT-symmetric

The Hamiltonian H and parity operator P take the following form

$$H = \begin{pmatrix} \omega_0 - i\gamma & \kappa \\ \kappa & \omega_0 + i\gamma \end{pmatrix}, P = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (A42)$$

Time-reversal operator T corresponds to complex conjugation.

We first calculate PH*P, which can be expressed as follows

$$PH^*P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \omega_0 + i\gamma & \kappa \\ \kappa & \omega_0 - i\gamma \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = H \quad (A43)$$

Since the time-reversal operator T and parity operator P satisfy T=T⁻¹ and P=P⁻¹, we rewrite above equation as

$$H^* = THT^{-1} = THT \quad (A44a)$$

$$H = PH^*P = PTHTP = (PT)H(PT)^{-1} \quad (A44b)$$

Rearranging Eq. A(44b) gives us

$$HPT = PTH \quad (45)$$

Therefore, Hamiltonian in Eq.(21) or Eq. A(42) is PT-symmetric. It also corresponds to the coupled system with equal gain and loss.

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