

From Local to Nonlocal High- Q Plasmonic MetasurfacesYao Liang¹, Din Ping Tsai^{1,2,3,*} and Yuri Kivshar^{4,†}¹Department of Electrical Engineering, City University of Hong Kong, Kowloon, Hong Kong SAR, China²State Key Laboratory of Terahertz and Millimeter Waves, City University of Hong Kong, Kowloon, Hong Kong SAR, China³Centre for Biosystems, Neuroscience and Nanotechnology, City University of Hong Kong, Kowloon, Hong Kong SAR, China⁴Nonlinear Physics Center, Research School of Physics, Australian National University, Canberra, Australian Capital Territory 2601, Australia

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The physics of bound states in the continuum (BICs) allows the design and demonstration of optical resonant structures with large values of the quality factor (Q factor) by employing dielectric structures with low losses. However, BIC is a general wave phenomenon that should be observed in many systems, including the metal-dielectric structures supporting surface plasmon polaritons where optical resonances are hindered by losses. Here we suggest and develop a comprehensive strategy to achieve high- Q resonances in plasmonic metasurfaces by effectively tailoring the resonant modes from local to nonlocal regimes, thus transitioning from quasi-isolated localized resonances to extended resonant modes involving strong interaction among neighboring structure metaunits.

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Introduction—Recent progress in metaphotonics is driven by the physics of optical resonances allowing us to achieve high values of the radiative quality factor (Q factor). One mechanism enabling high- Q dielectric metaphotonics is based on the physics of bound states in the continuum (BICs), which support sharp resonances for spatially localized modes within the continuum spectrum of extended states [1]. An ideal BIC in metasurfaces [2] is a dark state with an infinite lifetime that in practice always transforms into a quasi-BIC (qBIC) mode with finite Q manifested in the Fano effect. The study of BICs and qBICs has attracted much attention in recent years. The BIC concept has been employed for many problems requiring the enhancement of light-matter interaction with many applications including nanolasers [3,4], harmonic generation [5], biosensing [6], and optical imaging [7].

In a majority of applications, BICs are realized in dielectric photonic structures fabricated of materials with high value of refractive index [6–9], and the underlying physics explores the idea to reduce the radiative Q factor by adjusting geometric parameters, such as asymmetry of meta-atoms composing metasurfaces [2]. At the same time, several recent studies demonstrated the use of the BIC concept for hybrid metal-dielectric [10–12] and purely plasmonic [13–15] nanostructures.

We notice that the BIC concept relies on the basic principles of wave physics and wave interference [16]; thus, in general, it should be applied to both low-loss

dielectric and high-loss plasmonic structures. The main question is, what is the general strategy for engineering high- Q resonances in plasmonic structures? In this Letter, we uncover the basic physics underpinning high- Q plasmonic structures via the manipulation of dissipative properties of the resonant modes during the transition between local and nonlocal regimes in plasmonic metasurfaces. Here, “local” signifies quasi-isolated site resonances characterized by localized E fields and minimal mutual interaction among metaunits, whereas “nonlocal” indicates collective resonances with significantly extended E fields and strong interaction among metaunits.

Local to nonlocal transition in the parameter space—To illustrate our general strategy, first we focus on one recent example of a plasmonic metasurface (Fig. 1), consisting of vertical split-ring resonators (VSRRs) on a golden film substrate [13]. This plasmonic structure supports dark and

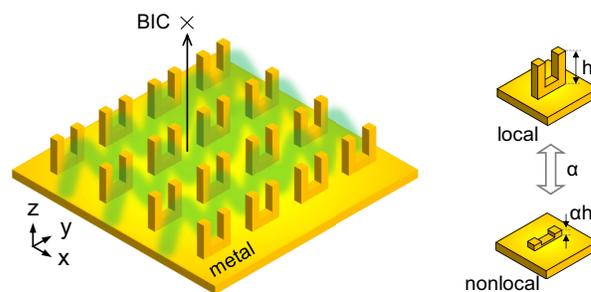


FIG. 1. Left: light trapping in a plasmonic (gold) BIC metasurface with vertical split-ring resonators. Right: transition between local and nonlocal resonances through the parameter scaling, with α being the scaling parameter.

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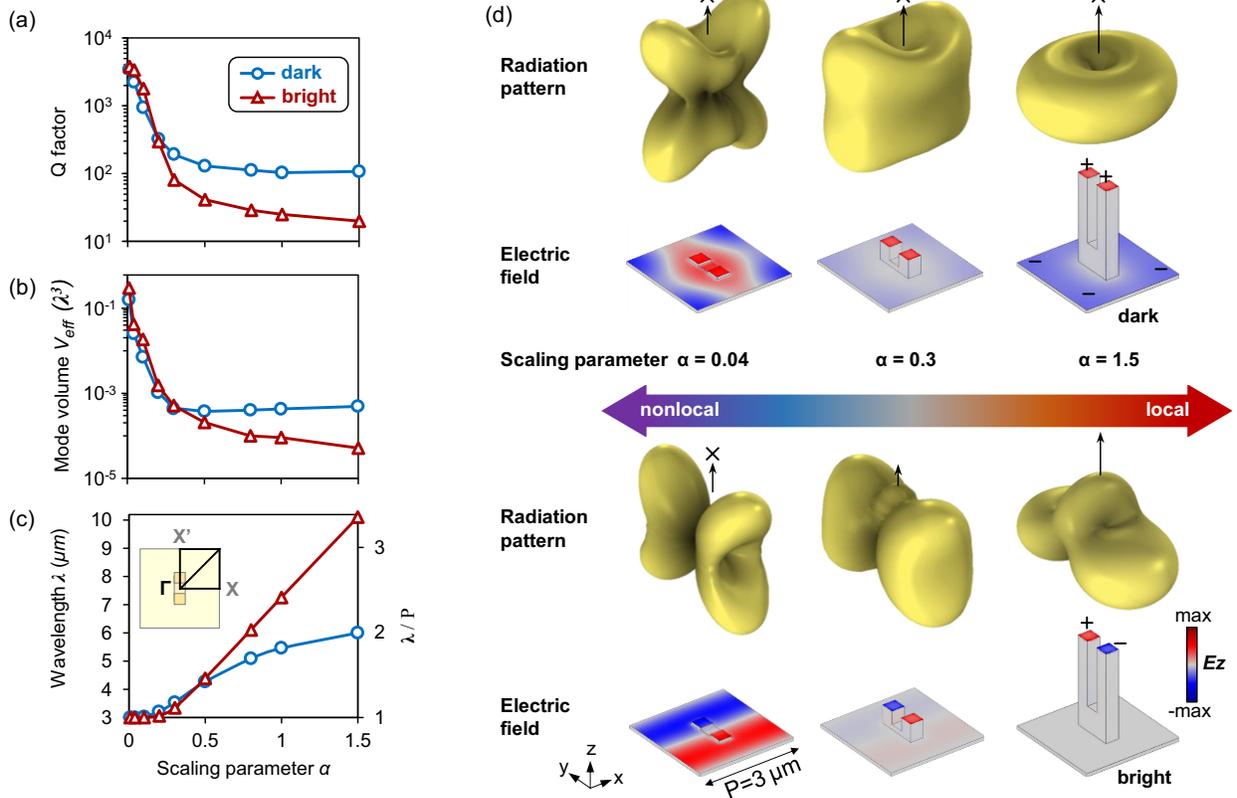


FIG. 2. Eigenmode analysis at the Γ point of VSRR metasurfaces. (a)–(c) The Q factor, mode volume, and resonance wavelength dependence on the scaling parameter α for the dark and bright modes. The initial parameters (at $\alpha = 1$) are period $3 \mu\text{m}$, square pillar width $0.4 \mu\text{m}$ and high $1.8 \mu\text{m}$, middle connector height $0.5 \mu\text{m}$, center-to-center distance between pillars $0.8 \mu\text{m}$. (c) Inset: Γ -point position. (d) The radiation patterns and electric fields (E_z) for various α .

bright localized surface plasmon resonances (LSPRs). The initial geometric parameters are shown in the caption of Fig. 2. By exclusively scaling the height parameters (the pillars and middle-connector heights) with the scaling factor α while keeping other parameters constant, it facilitates a transition between local and nonlocal regimes for both the modes. Here, $\alpha > 1$ indicates an increase, while $\alpha < 1$ indicates a decrease.

Figure 2 illustrates this transition in parameter space at the Γ point of arrays, specifically, at the in-plane emission wave vector $k_{\parallel} = (k_x, k_y) = 0$, where k_x and k_y denote the wave vector components along the x and y axes. We categorize odd and even symmetry LSPRs, corresponding to in-plane and out-of-plane resonances, as bright and dark modes based on their far-field radiation at local regimes. Decreasing the scaling parameter α from 1.5 to 0.01 leads to a shift from local to nonlocal resonance with two notable features: (1) the resonance wavelengths (in free space) approach the period ($\lambda \rightarrow P$, where $P = 3 \mu\text{m}$), as shown in Fig. 2(c); (2) a significant increase in Q factor [Fig. 2(a)], and mode volume [Fig. 2(b)] for both modes, with differences spanning several orders of magnitude. The Q factor is calculated using $Q = \omega_r / 2\omega_i$, where ω_r and ω_i are the real and imaginary parts of eigenfrequencies.

In pure local regimes, when $\alpha = 1.5$, the bright LSPR mode, for example, exhibits a resonance wavelength ($\lambda \sim 10 \mu\text{m}$) several times larger than the lattice period ($P = 3 \mu\text{m}$), as shown in Fig. 2(c). The individual unit resonance (local) prevails in this local LSPR, overshadowing negligible contributions from collective resonances (nonlocal) that depend on strong interactions among neighboring units [17]. This is evident because a single isolated unit exhibits a nearly identical electric field profile and spectral enhancement as the entire array [see Supplemental Material (SM) [18], S3].

However, the Q factor for the bright LSPR is low, $Q \approx 19.8$ at $\alpha = 1.5$ [Fig. 2(a)]. This is predominantly attributed to two reasons.

First, its tight light confinement, evident through hot spots on the tops of pillars [Fig. 2(d)] and an ultrasmall mode volume (SM [18], S2) well below the diffraction limit [$V_{\text{eff}} \sim 5.13 \times 10^{-5} \lambda^3$, Fig. 2(b)]. These hot spots amplify the electric field ($|\mathbf{E}|$), causing a notable increase in the metal's dissipation density, $w = 1/2\epsilon_0 \text{Im}(\epsilon) |\mathbf{E}|^2$, where ϵ_0 and $\epsilon = \epsilon_r + i\epsilon_i$ denote the vacuum permittivity and relative permittivity of gold. This giant dissipation loss hampers sustaining light energy exchange between the E field and the H field, preventing high- Q resonances. The reason is

simple: high- Q resonances, known for long-lasting light oscillation in cavities, require a sustaining oscillation between electric field energy ($u_E \propto \epsilon \mathbf{E}^2$) and magnetic field energy ($u_H \propto \mu \mathbf{H}^2$) in a cavity due to light's electromagnetic nature, where μ is the permeability [41]; Once giant E -field or H -field hot spots present, this sustaining oscillation is damaged, leading to low- Q resonances.

Second, it has giant radiation loss. In plasmonic cavities, their resonance Q factor reads

$$Q^{-1} = Q_{\text{rad}}^{-1} + Q_{\text{dis}}^{-1}, \quad (1)$$

where Q_{rad} and Q_{dis} are, respectively, the radiation and dissipation Q factors. See SM [18], S1 for simulation and calculation details.

One way to improve the LSPR Q factor is to suppress radiation loss using dark modes with $Q_{\text{rad}} = \infty$. The Q factor for the dark LSPR is $Q \approx 107.8$ at $\alpha = 1.5$ [Fig. 2(a)], representing a $5\times$ improvement over the bright LSPR. This improvement is also attributed to the nonlocality of the dark LSPR. Notably, the resonance wavelength of the dark LSPR ($\lambda_{\text{dark}} \approx 6 \mu\text{m}$) is significantly smaller than that of its bright counterpart ($\lambda_{\text{bright}} \approx 10 \mu\text{m}$). A shorter resonance wavelength enhances nonlocality (see latter discussion and SM [18], S3).

While purely local resonances are limited to isolated plasmonic particles, all resonances in plasmonic arrays exhibit nonlocality due to coupling between neighboring metaunits, resulting in suppressed in-plane radiation (SM [18], S3). In this study, we refer to dark and bright modes in plasmonic arrays with large height scaling parameters (e.g., $\alpha = 1.5$) as local resonances for simplicity, as they are primarily driven by LSPRs. More accurately, these modes should be termed quasi-isolated localized modes.

However, the dark LSPR's Q factor is limited by significant dissipation loss linked to strong local light confinement, observed as hot spots on pillar tops [Fig. 2(d)].

Utilizing our local-to-nonlocal transition strategy effectively minimizes dissipation loss. In this transition, the E field becomes less confined and extends more into the lossless air (SM [18], S4). This is accomplished by increasing mode volumes [Fig. 2(b)] and the gradual disappearance of hot spots on pillar tops, eventually resulting in a uniformly distributed E -field profile on the gold film plane [Fig. 2(d)]. These features substantially reduce resonances' dissipation loss, as indicated by large Q factors, $Q \approx 3439$ (dark) and $Q \approx 3802$ (bright) at $\alpha = 0.01$ for both modes [Fig. 2(a)], several orders of magnitude larger than the local LSPRs. These high- Q nonlocal modes are collective resonances strongly coupled with nonlocal diffraction orders.

Diffraction orders and nonlocality—Collective resonance modes in a plasmonic array can be decomposed into Bloch harmonics [42], given by $\mathbf{E}(\mathbf{r}) = \sum a_{(p,q)} e^{-i(k_{\parallel} + pG_x + qG_y)\mathbf{r}}$, where $a_{(p,q)}$ is the complex amplitude, k_{\parallel} the in-plane k vector, $G_x = (2\pi/P_x)\hat{x}$ and $G_y = (2\pi/P_y)\hat{y}$ the array reciprocal vectors, with the metaunit periods $P_x = P_y = P = 3 \mu\text{m}$ and $p, q \in \mathbb{Z}$.

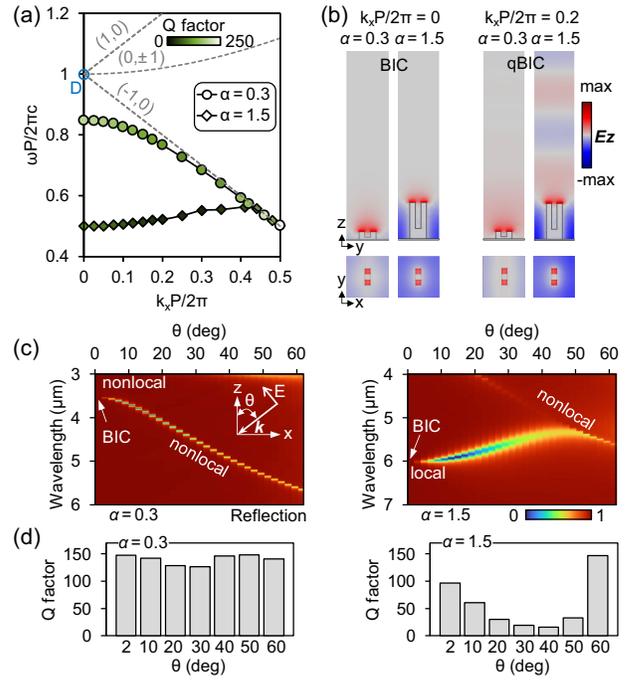


FIG. 3. (a) Calculated band structure for the dark mode with nonlocal ($\alpha = 0.3$) and local ($\alpha = 1.5$) characteristics, denoted by circular and square markers, respectively. The color represents eigenmode Q factor. The gray dashed lines represent three diffraction orders: (1,0), (-1,0), and (0,±1). The blue circle denotes the D point. (b) The field distribution of dark modes for two metasurfaces ($\alpha = 0.3$ and $\alpha = 1.5$) at $k_x P/2\pi = 0$ (Γ point) and $k_x P/2\pi = 0.2$ (off Γ). (c) Reflection spectra for two metasurfaces ($\alpha = 0.3$ and $\alpha = 1.5$) at oblique incidence in the x - z plane under TM polarized light excitation (E -field vector in the incident plane). (d) The corresponding Q factor of the two dark modes at different oblique angles. The Q factor is the ratio of resonance wavelength to full width at half maximum.

The empty lattice dispersion equation $|k_{\parallel} + pG_x + qG_y| = 2\pi/\lambda$ defines momentum space positions where propagating diffraction orders (p, q) emerge [gray dashed lines, Fig. 3(a)]. Specifically, at the Γ point of the array, we identify a highly symmetric position termed the D point [blue circle in Fig. 3(a)], where three diffraction orders (1,0), (-1,0), and (0,±1) degenerate. We assign the corresponding operational wavelength $\lambda_D = P$ as the degenerate wavelength.

At Γ -point direction, D point is a critical transition point. Specifically, the Bloch harmonics (1,0), (-1,0), (0,±1) can either exist as bounded evanescent waves when $\lambda > \lambda_D$ or transform into propagating diffraction orders when $\lambda < \lambda_D$. At $\lambda = \lambda_D$ those harmonics travel along the array surface at a grazing angle and interact with many metaunits (nonlocality). We use normalized detuning wavelength (Δ) to describe the distance between resonance wavelength λ and λ_D :

$$\Delta = \frac{\lambda - \lambda_D}{\lambda_D} = \frac{\lambda - P}{P}. \quad (2)$$

As Δ decreases approaching zero, LSPRs transition into collective resonances dominated by surface plasmon polaritons (SPPs), (SM [18], S4). LSPRs exhibit strong light confinement (hot spots) and weak interunit coupling. Conversely, SPPs have significantly extended E fields into the air due to strong interaction with nonlocal diffraction orders. This explains the larger mode volumes of nonlocal modes compared to local LSPRs [Fig. 2(b)].

Nonlocal nature of modes—The high- Q nonlocal modes are trapped SPPs, characterized by standing SPP waves confined in a Fabry-Perot cavity (SM [18], S4 and S5). Two pieces of evidence support this interpretation.

First, trapped SPPs exhibit no far-field radiation. Consequently, all nonlocal plasmonic modes, whether transitioning from a dark or bright LSPR in the local to nonlocal shift, should remain subradiative if they are trapped SPPs. The dark LSPR supports this characteristic throughout the transition [Fig. 2(d)]. Interestingly, despite being radiative in local regimes ($\alpha = 1.5$), the bright LSPR becomes less radiative ($\alpha = 0.3$) and eventually becomes radiation-free in nonlocal regimes ($\alpha \leq 0.04$) [see Fig. 2(d) and S4 in SM [18]]. This aligns with the dark feature of trapped SPPs. See S8 in SM [18] for radiation pattern understanding. Second, another evidence is linked to the Q -factor limit of the nonlocal mode.

Q-factor limit—As Δ decreases, dark and bright LSPRs shift into trapped SPPs, exhibiting minimal dissipation loss, enabling efficient energy exchange between E field and H field. To determine the upper limit of Q factors for nonlocal plasmonic resonances, we can assess

$$Q_{\max} = \frac{k_{\text{SPP}}^r}{2k_{\text{SPP}}^i}, \quad (3)$$

where k_{SPP}^r and k_{SPP}^i are the real and imaginary part of SPP's k vector, such that $k_{\text{SPP}} = k_{\text{SPP}}^r + ik_{\text{SPP}}^i = (2\pi/\lambda)\sqrt{[\epsilon\epsilon_0/(\epsilon + \epsilon_0)]}$, where ϵ and ϵ_0 are the permittivities of gold and vacuum [43]. As ϵ varies with wavelength, the maximum Q factor of nonlocal plasmonic resonance is wavelength dependent (SM [18], S6). For $\lambda \approx 3 \mu\text{m}$, the trapped SPP's Q factor is calculated as ~ 3805 , consistent with numerical results of nonlocal mode in Fig. 2(a).

Local-nonlocal transition in the momentum space—The local-to-nonlocal transition can also occur in the momentum space as the resonance modes interact with nonlocal diffraction orders. For example, we calculate the eigenfrequency and Q factor for two dark modes with different height parameters, $\alpha = 1.5$ (local) and $\alpha = 0.3$ (nonlocal); see Fig. 3(a). They are symmetry-protected BICs with zero radiation loss at the Γ point ($k_{\parallel} = 0$); see Fig. 3(b) (left). As the in-plane vector $k_x = (\omega/c)\sin(\theta)$ increases, BICs transit to qBICs with two distinguished properties.

First, the Q factor of the local qBIC mode experiences a rapid decrease, whereas the Q factor of the nonlocal qBIC mode remains stable, as verified by both eigenmode studies

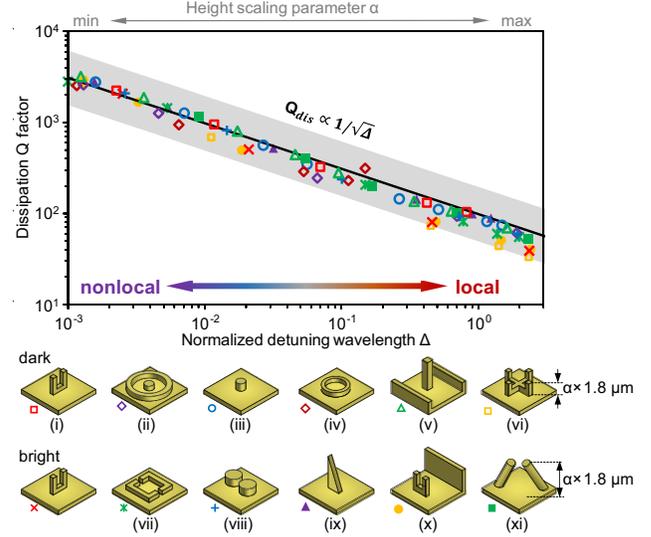


FIG. 4. Dependence of the dissipation Q factor on the normalized detuning wavelength Δ (log-log scale) for various all-plasmonic designs [(i)–(xi)] supports bright and dark LSPRs (Refs. [13–15,44–51]) All square units have a $3 \mu\text{m}$ period.

[Fig. 3(a)] and full-wave simulations [Figs. 3(c) and 3(d)]. This results from different coupling strengths between the two modes and diffraction order $(-1, 0)$. For example, the resonance frequency of nonlocal mode is closer to diffraction order $(-1, 0)$ than its local counterpart at $k_x P/2\pi = 0.2$. Thus, it relies more on the mutual interaction among neighboring units, which reduces its radiation loss [17]. This makes it less radiative compared to the local counterpart [Fig. 3(b), right]. Also, its nonlocal feature makes it less dissipative. These two features help it keep high- Q resonances at various oblique incidences [Figs. 3(c) and 3(d)].

Second, the local mode becomes nonlocal at large oblique incidence angles ($\theta > 40^\circ$) as it approaches $(-1, 0)$ diffraction order [Fig. 3(c)]. This is evident by a sudden increase in its Q factor when $\theta > 40^\circ$ [Fig. 3(d)].

Local-nonlocal transition in plasmonic metasurfaces—Our approach to improving the Q factor in plasmonic nanostructures by reducing the height parameter is not limited to a specific metasurface with VSRR units. Instead, it is a universally applicable strategy that can be employed for all types of plasmonic metasurfaces with various metaunits, including single pillar, ring, dimmer, triangular prism, pillar wall, and many others [13–15,44–51], as shown in Fig. 4.

All metasurfaces in Fig. 4 support LSPRs. For simplicity, we set them as square units with a $3 \mu\text{m}$ period and an initial height of $1.8 \mu\text{m}$ ($\alpha = 1$). They have the same degenerate wavelength $\lambda_D = P = 3 \mu\text{m}$. As the height scaling parameter α decreases, LSPRs (dark or bright) transition into trapped SPPs with similar, symmetric or antisymmetric, E -field profiles (SM [18], S7).

We study the dependence of the dissipation Q factor Q_{dis} on the normalized detuning wavelength Δ for all plasmonic metasurfaces during the local (LSPRs) to nonlocal (trapped SPPs) transition (Fig. 4). An inverse square root law well approximates the relationship,

$$Q_{\text{dis}} \propto \frac{1}{\sqrt{\Delta}}, \quad (4)$$

where Δ is calculated using Eq. (2), and Q_{dis} using Eq. (1) (SM [18], S1). Notably, in pure nonlocal regimes ($\Delta \sim 10^{-3}$), the Q factor ($Q = Q_{\text{dis}}$ as $Q_{\text{rad}} = \infty$) of all plasmonic metasurfaces is approaching ~ 3800 , consistent with prediction using Eq. (3), confirming the trapped SPPs nature of the nonlocal modes.

The inverse square root law suggests an intelligent way to engineer plasmonic structures with on-demand resonance Q factor. Most resonances have hybrid (LSPRs + SPPs) properties during the local-to-nonlocal transition. For example, at $\alpha = 0.3$, the bright mode has both hot spots on pillars' tops (local LSPR feature) and trapped SPPs (nonlocal) on the ground plane [Fig. 2(d)]. Notably, hot spots [52] and high- Q resonances [13] are effective ways to enhance the electromagnetic field. A maximum E -field intensity occurs at some point during this transition (SM [18], S3), which proves beneficial for applications such as nonlinear enhancement [53] and fluorescence enhancement [54].

Equation (4) holds for a broad range, $\Delta \in [10^{-3}, 1]$, allowing diverse Q -factor choices (tens to thousands) for most plasmonic metasurfaces. However, plasmonic Q factors are inherently limited, approaching that of trapped SPPs [Eq. (3)]. Achieving higher Q factors in nonlocal regimes necessitates scaling up the lattice period to extend the operational wavelength, as the maximum Q factor is wavelength dependent. This is shown by $Q_{\text{max}} \sim 627$ at $\lambda = 880$ nm and $Q_{\text{max}} \sim 6330$ at $\lambda = 5$ μm (SM [18], S6). This wavelength-dependent trend aligns with recent experimental results ($Q \sim 80$ in near IR [44] and $Q \sim 500$ in mid-IR [55]).

Conclusion—We have suggested a general conceptual approach for achieving large Q factors in plasmonic metastructures by engineering dissipation Q factor of the resonant modes. Our approach employs an efficient control of local and nonlocal optical response, and it is underpinned by the physics of bound states in the continuum. We believe the suggested strategy may open the door to many novel applications of plasmonic structures including efficient lasing, harmonic generation, biosensing, optical imaging, and entangled photon generation.

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