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Strong coupling between excitons in transition metal dichalcogenides and optical bound states in the continuum

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Abstract. Being motivated by recent achievements in the rapidly developing fields of optical bound states in the continuum (BICs) and excitons in monolayers of transition metal dichalcogenides, we analyze strong coupling between BICs in Ta_2O_5 periodic photonic structures and excitons in WSe_2 monolayers. We demonstrate that giant radiative lifetime of BICs allows to engineer the exciton-polariton lifetime enhancing it three orders of magnitude compared to a bare exciton. We show that maximal lifetime of hybrid light-matter state can be achieved at any point of **k**-space by shaping the geometry of the photonic structure.

1. Introduction

Monolayers of transition metal dichalcogenides (TMDCs) are a certain class of post-graphene two-dimensional materials, attracting vast research interest in recent years. Excitons in TMDC monolayers shows variety of unique features, such as large binding energy [1], leading to strong excitonic response at room temperature, and significant oscillator strength, providing substantial exciton-photon interaction. These properties allow the observation of the so-called strong coupling regime, leading to the emergence of the new quasiparticles, exciton-polaritons [2] even at room temperatures [3].

Strong coupling of TMDC excitons with light has been observed in the structures resembling the conventional microcavities, where the monolayer has been sandwiched between two Bragg mirrors. However, since fabrication of hight quality TMDC monolayers is based on mechanical exfoliation techniques, with are not compatible with the standard epitaxial techniques used for the Bragg mirror fabrication, the realisation of structures supporting exciton-polaritons is quite technologically demanding.

In this work we suggest using photonic crystal slab, supporting optical bound states in the continuum (BICs), to achieve strong exciton-photon coupling. BICs demonstrate exceptional properties [4], in particular, giant radiative lifetime, limited only be surface roughness, and could be excited by plane wave, what favourably distinguishes them from waveguide modes.

2. Results

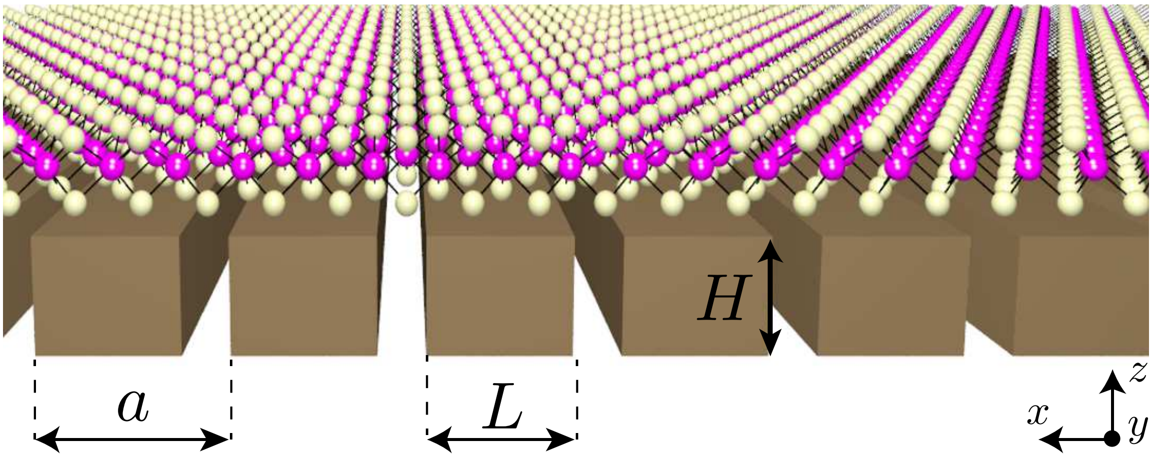

Figure 1. (a) Sketch of a studied structure. The refractive index of Ta_2O_5 bars $\varepsilon = 2.1$. The TMDC made of WSe_2 is laid on top of the PhC slab. The calculations performed for the PhC with period $a = 1.03H$ and bars width $a = 0.9L$

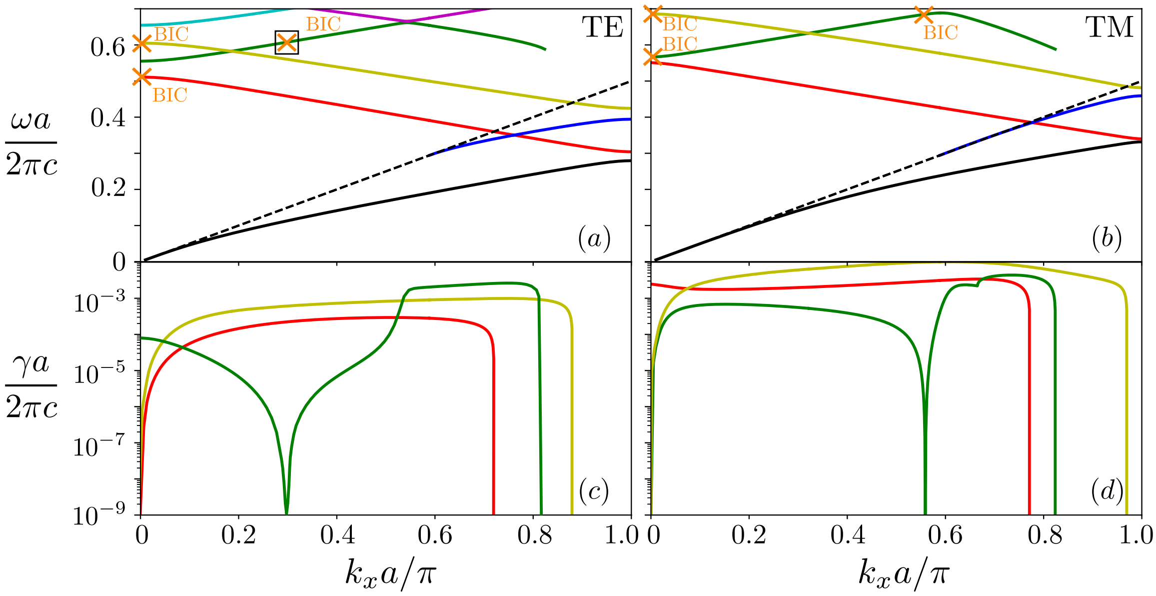

Figure 2. Eigenmode spectrum of air-suspended Ta_2O_5 one-dimensional grating. Band structure for (a) TE-polarized and (b) TM-polarized modes, respectively. Dimensionless inverse radiation lifetime for (c) TE-polarized and (d) TM-polarized modes, respectively. BICs are marked by orange crosses.

We use the guided-mode expansion [5] method to obtain exciton photonic crystal slab (PCS) eigenmodes. Photonic crystal slab consists of Ta_2O_5 rectangular bars with height H and width L being spaced equidistant with period a. We put refractive index of Ta_2O_5 equal to 2.1 which is appropriate for the red band of the visible spectrum range [7]. The calculation are performed for PCS with $a = 1.03H$, $L = 0.9a$. The spectrum of eigenfrequencies and inverse radiation lifetimes of the PCS for in-plane wavevectors along the x direction of the first Brillouin zone is shown in Fig. 2(a,c) for TE-polarized, Fig. 2(b,d) for TM-polarized modes, respectively. Dispersion curves under the light line $\omega = ck_x$ describe pure guided modes with zero diffraction losses while photonic states above the light line are leaky provided their radiation lifetime is finite. The BICs represent unusual leaky modes with $\gamma = 0$ and can be formed both at the center of the Brillouin zone (at-Γ BIC) and at specific points between the zone edge and center (off-Γ BIC).

In order to tune the off-Γ BIC frequency to a resonance with exciton energy $E_{exc} = 1.74$ eV [6] PCS hight equal to $H = 418$ nm was taken. Fig. 3(a) demonstrates strong coupling between the exciton and the off-Γ BIC which manifests itself as an avoided resonance crossing with Rabi splitting of order of 3 meV. Exciton-polariton inverse lifetime are shown in Fig. 3(b) in comparison with the inverse lifetimes of bare excitonic and photonic modes. As it can be seen, for specific values of k_x the lifetime of polariton modes can exceed the bare exciton lifetime by almost three orders of magnitude and reaches 0.66 ns. The most important, Fig. 3(b) shows the maximal lifetime can be realized not at the center or the edge of the Brillouin zone,but at the pointof phase space,where the group velocity of the mode is finite.

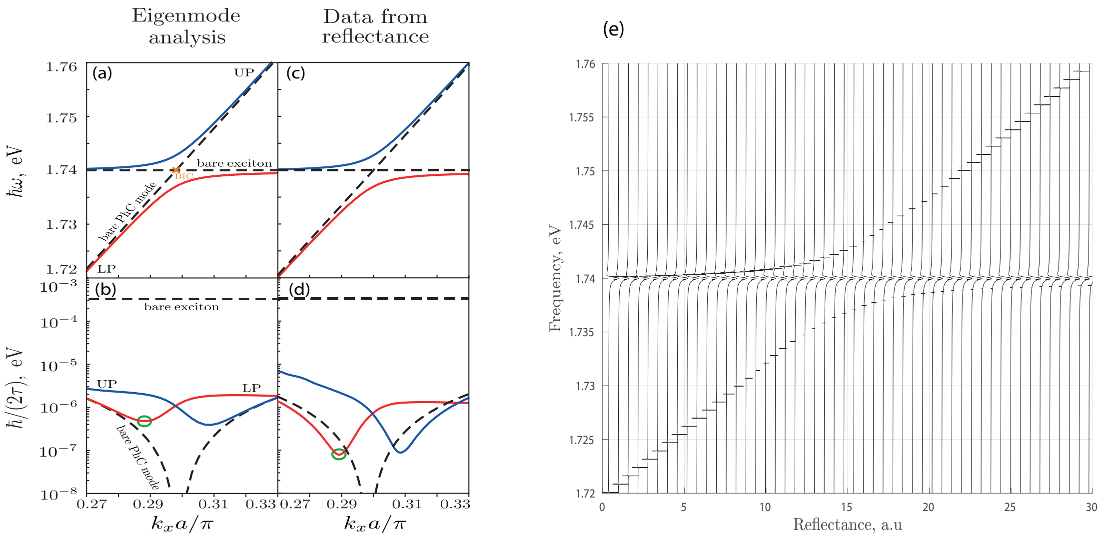

Figure 3. Dispersion and inverse lifetime of exciton-polaritons at the conditions of strong coupling between the TE-polarized photonic mode supporting an off-Γ BIC and in-plane polarized exciton (a,b) and the fitting of Fano lineshape of reflection spectrum (c,d). (e) Reflectance spectrum of WSe_2 placed on top of photonic crystal slab. Each spectrum is shifted in horizontal dirction by 0.6

The reflectance spectrum, which could be experimentally observed using angle-resolved reflection spectroscopy, was obtained via using Fourier modal method [8] is shown in Fig. 3(e). We fit the reflectance spectrum to Fano lineshape using Levenberg-Marquardt algorithm to obtain real and imaginary parts of eigenfrequency shown in Fig. 3(c,d). We see that the GME method and the reflectance spectrum calculations show good agreement providing the same value of Rabi splitting and the 3-fold enhancement of LP lifetime with respect to a bare exciton. However, the maximal values of the damping rate extracted by the fitting method are one order smaller than those for the eigenmode analysis. The difference is the result of approximations used for the GME calculations.

Finally, we calculate the dependence of lower-polariton lifetime on in-plane wavevector $\boldsymbol{k} = k_x, k_y$ in the two-dimensional Brillouin zone by means of the eigenmode analysis. One can see that lifetime value exhibits maximum at $k_x \pm 0.29\pi/a$, $k_y = 0$ and decreases smoothly in the vicinity of these points.

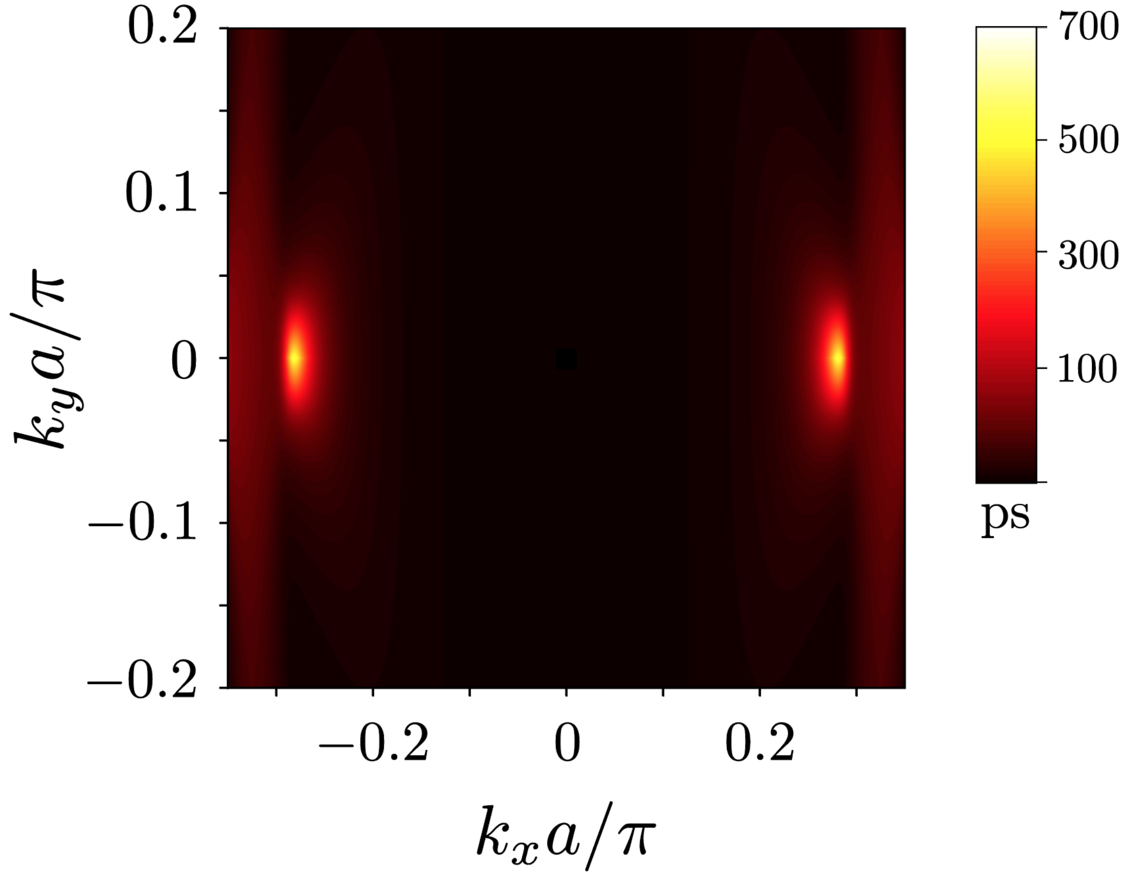

Figure 4. Map of dependence of lifetime of the lower polariton mode on in-plane wavevector.

3. Conclusion

We have proposed an experimentally feasible scheme to achieve strong coupled exciton-photon system in a two-dimensional nanostructure comprising a TMDC monolayer and a periodic photonic nanostructure. Importantly, this scheme does not require the growth of Bragg mirrors, which substantially simplifies the fabrication. Moreover, we have shown that it also allows the polariton condensation at the finite momenta, which opens possibilities for the non-resonant excitation of moving polariton condensates

Acknowledgements

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