Screening and plasmons in pure and disordered single- and bilayer black phosphorus

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Introduction

Phosphorene is a new kind of two-dimensional (2D) material that can be obtained by the mechanical exfoliation method from black phosphorus (BP) films. We study screening and collective plasmon excitations of pure and disordered single- and bilayer BP beyond the low energy continuum approximation by using a tight-binding (TB) model which properly accounts for the electronic band dispersion in a wide energy window. The effects of disorder on the electronic and optical properties of this material are addressed.

Tight-binding model

BP is a single-elemental layered crystalline material consisting of only phosphorus atoms arranged in a puckered orthorhombic lattice (Fig. 1). The electronic band structure around the gap can be described with a TB Hamiltonian for pristine BP with the form [1]

$$H = \sum_i \epsilon_i n_i + \sum_{i \neq j} t_{ij} c_i^+ c_j + \sum_{i \neq j} t_{p,ij} c_i^+ c_j ,$$

where we consider five intralayer and four interlayer hopping terms.

We consider two main different sources of disorder in BP: local point defects (resonant scatterers, RS) and long-range disorder potential (LRDP). The amount of RS and LRDP are quantified by n_x and n_c.

Numerical method

The dynamic polarization function is obtained from the Kubo formula, which is explicitly written as [2]

$$\Pi(q,w) = -\frac{2}{V}\int_0^\infty d\tau\, e^{i\omega\tau} \mathrm{Im}\,\langle\varphi|n_F(H)e^{iH\tau}\rho(q)e^{-iH\tau}[1-n_F(H)]\rho(-q)|\varphi\rangle,$$

where $\rho(q)$ is the density operator, $n_F(H) = \frac{1}{e^{\beta(H-\mu)}+1}$ is the Fermi-Dirac distribution operator, and $|\varphi\rangle$ is a random wave function.

We introduce two time evolutions of the random wave function:

$$|\varphi_1(q,\tau)\rangle = e^{-iH\tau}[1-n_F(H)]\rho(-q)|\varphi\rangle,$$
$$|\varphi_2(\tau)\rangle = e^{-iH\tau}n_F(H)|\varphi\rangle,$$

which allows us to express the real and imaginary part of the dynamic polarization as

$$\mathrm{Re}\Pi(q,w) = -\frac{2}{V}\int_0^\infty d\tau \cos(\omega\tau)\,\mathrm{Im}\,\langle\varphi_2(\tau)|\rho(q)|\varphi_1(q,\tau)\rangle,$$

$$\mathrm{Im}\Pi(q,w) = -\frac{2}{V}\int_0^\infty d\tau \sin(\omega\tau)\,\mathrm{Im}\,\langle\varphi_2(\tau)|\rho(q)|\varphi_1(q,\tau)\rangle.$$

Electron-electron interactions are considered within the random phase approximation (RPA). The two-dimensional dielectric function for single-layer BP is calculated as

$$\varepsilon_{1L}(q,\omega) = 1 - V(q)\Pi(q,\omega),$$

where $V(q) = \frac{2\pi e^2}{\kappa q}$ is the Fourier component of the Coulomb interaction in two dimensions, in terms of the background dielectric constant κ.

The dielectric tensor of bilayer BP is expressed as

$$\varepsilon_{2L}(q,\omega) = \begin{pmatrix} \varepsilon_{1L}(q,\omega) & -V(q)F(q)\Pi(q,\omega) \\ -V(q)F(q)\Pi(q,\omega) & \varepsilon_{1L}(q,\omega) \end{pmatrix},$$

where $F(q) = e^{-qd}$ and d is the interlayer distance.

Simulation results (2): Plasmons

The collective modes (plasmon) of the system are defined by the zeros of the dielectric function $\varepsilon(q,\omega)$, which leads to poles in the energy loss function $-\mathrm{Im}1/\varepsilon(q,\omega)$.The results are shown in Fig. 3 (single-layer) and Fig. 4 (bilayer).

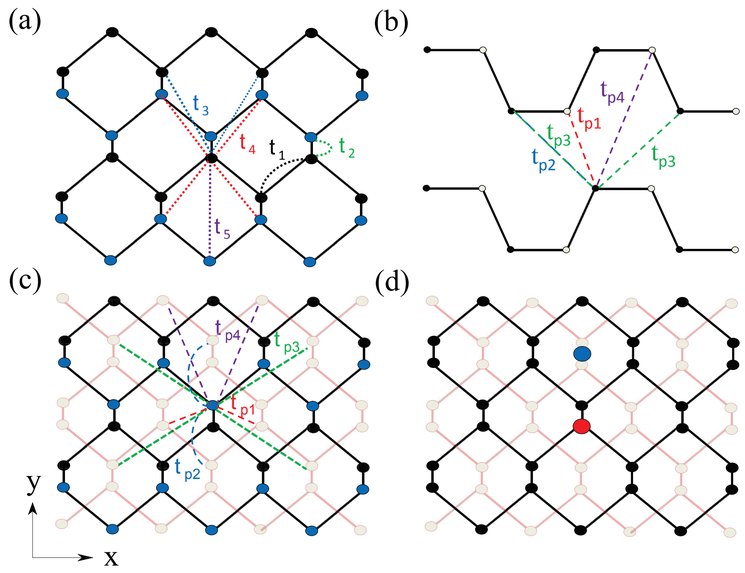

Fig. 1. Lattice structure of single- and bilayer BP.

Simulation results (1): Dielectric screening

In Fig. 2, we plot the static dielectric function $\varepsilon(q,0)$ of single- and bilayer BP. There is a clear dependence of the static dielectric function with the direction of momentum, showing a different behavior for q along the zigzag (x) or armchair (Y) directions.

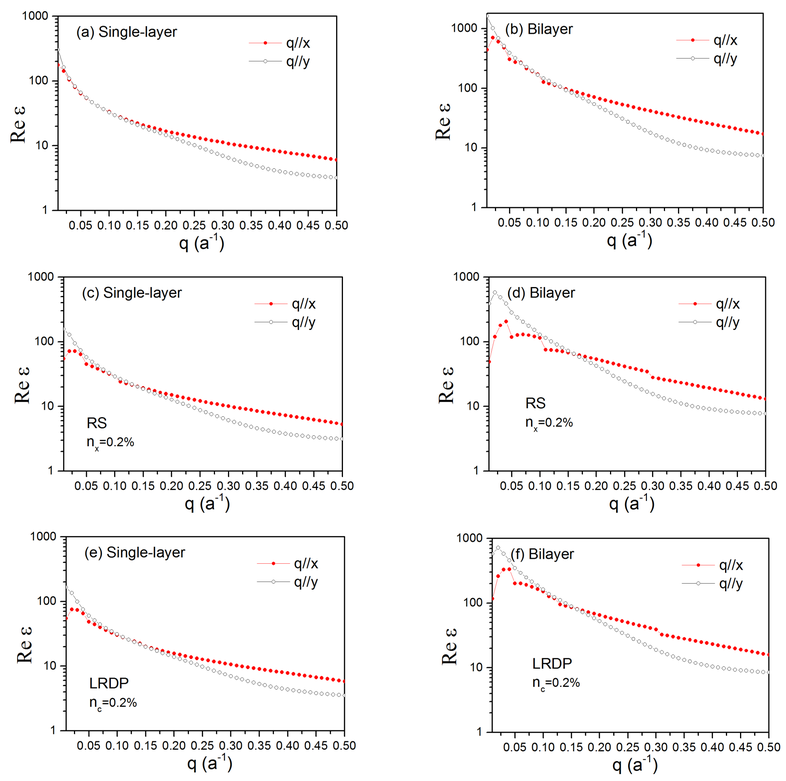

Fig. 2. Static dielectric function of single- and bilayer BP.

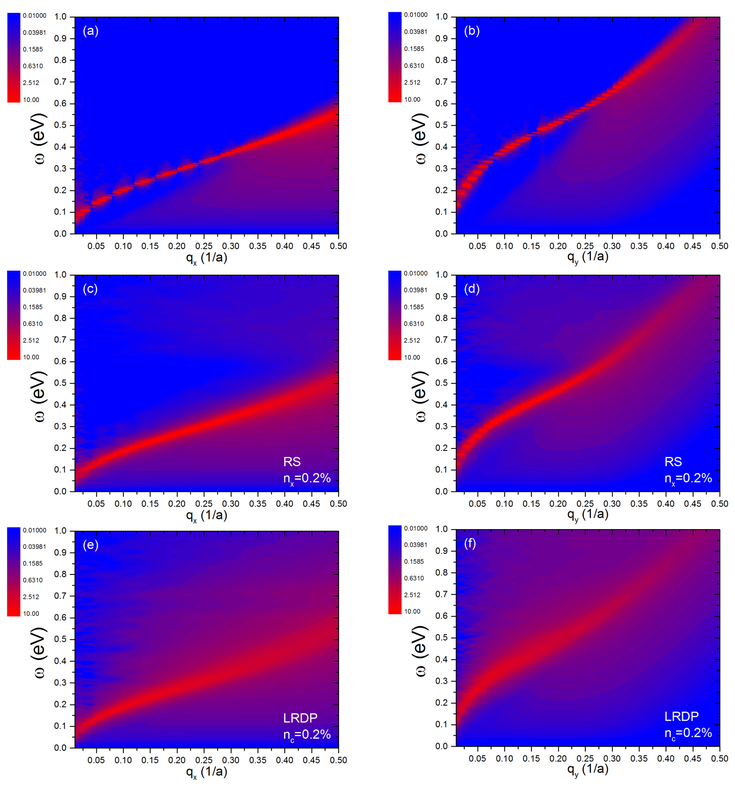

Fig. 3. Energy loss functions of single-layer BP along zigzag and armchair directions.

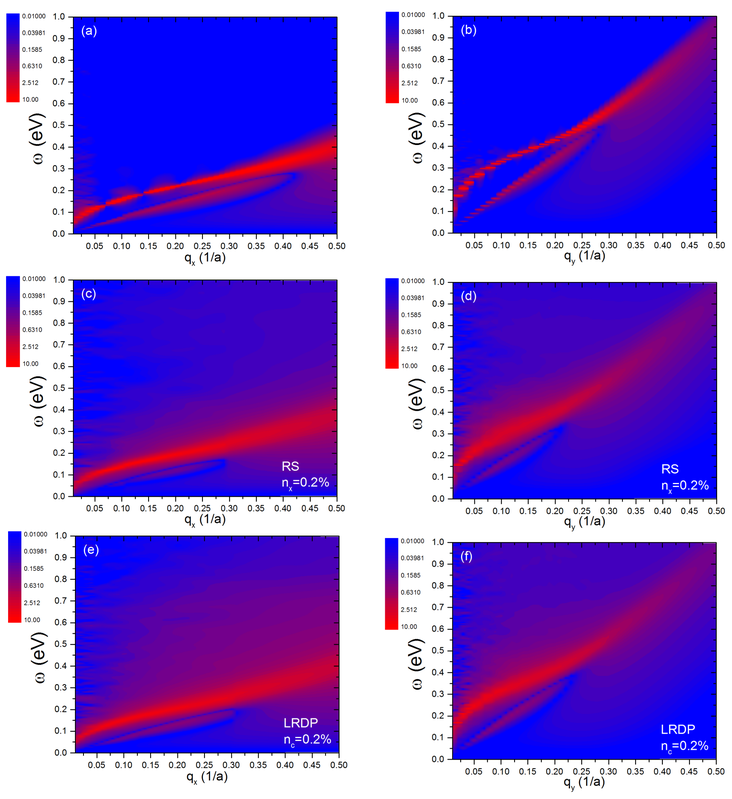

Fig. 4. Energy loss functions of bilayer BP along zigzag and armchair directions.

Summary

We have studied the effect of disorder in the excitation spectrum of single- and bilayer BP. The dynamical polarization function has been calculated with the Kubo formula, and from this, the energy loss function has been obtained within the RPA. We have found that disorder leads to a redshift of the plasmon resonance. More results and discussions can be found in Ref. [3]

Reference:

[1] A. N. Rudenko and M. I. Katsnelson, Phys. Rev. B **89**, 201408 (2014).

[2] S. Yuan, R. Roldán, and M. I. Katsnelson, Phys. Rev. B 84, 035439 (2011)

[3] F. Jin et al, Phys. Rev. B **92**, 115440 (2015).