Electronic and Optical Properties of Plasmonic Topological Insulators

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Topological insulator (TI) crystals are bulk insulators with robust conducting surface states protected by time-reversal symmetry due to strong spin-orbit coupling (SOC). These TI materials have been widely investigated for spintronic applications and quantum computation [1], and now are considered emerging optical materials for surface plasmonics [2]. Among these TI materials, $Bi_{2-x}Sb_xTe_{3-y}Se_y$ (BSTS) shows superior properties of large bulk resistance and surface-dominated transport, as well as negative permittivity and low-loss plasmonic resonances in the visible part of the spectrum [3].

Here we present a theoretical study on the electronic band structures and dielectric functions of various topological insulator materials by first-principle calculations based on many-body perturbation theory. Both random phase approximation (RPA) and Bethe-Salpeter equation (BSE) methods were employed to calculate the dielectric functions. The optimized lattice parameters of BSTS by using our generated realistic pseudopotentials reproduce well the experimental crystal structures. As shown in Fig 1a, the bulk band structures show an inversion between the conduction band and valence band at Γ point due to band splitting. By increasing the strength of SOC, the direct bandgap becomes indirect, allowing strong optical transitions around the Z region. In Fig 1b, the negative regime of real part in calculated dielectric function arises from allowed interband dipole transitions at Γ point or Z region including SOC effects. The cross bulk plasma wavelength can be tuned in the visible and near-infrared regime by adjusting the composition of BSTS. Interestingly, the lager dielectric constant can be achieved by increasing ratio of Te element, a valuable design parameter for the synthesis of new TI compounds.

In summary, we determined electronic and optical properties of topological insulator BSTS crystals by first-principle calculations. Our results elucidate origin and composition dependence of bulk plasma wavelength in the visible and near-infrared parts of the spectrum and provide a solid framework to screen out BSTS and other TI compounds to design optical and plasmonic properties on demand.

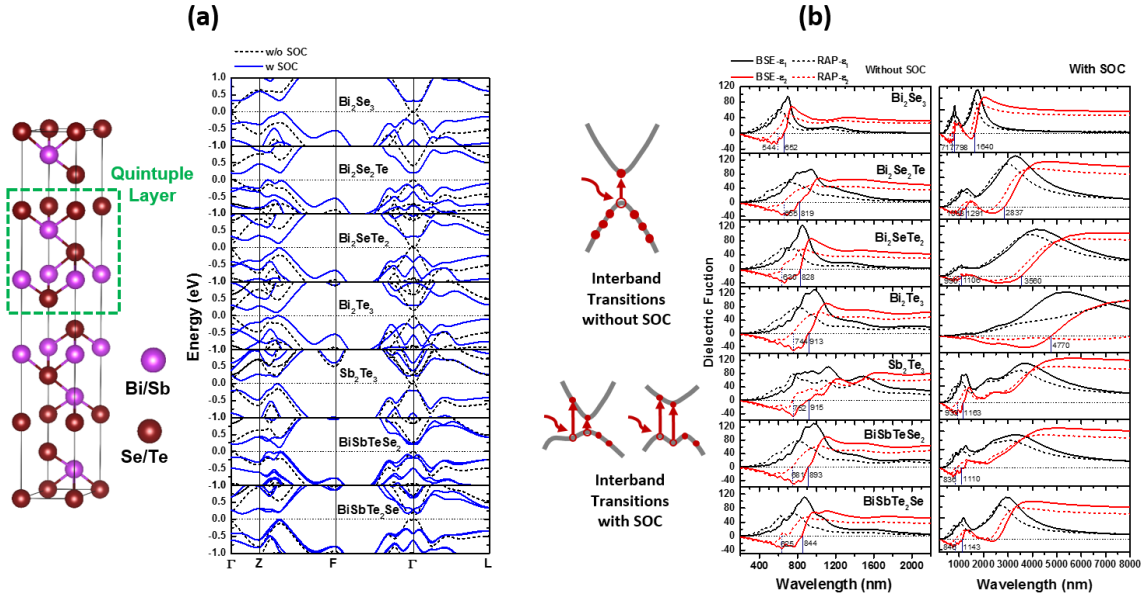

Fig. 1 (a) Crystal and electronic band structure of BSTS obtained by DFT-LDA and DFT-LDA-SOC method; (b) Optical properties of BSTS calculated by BSE and RAP methods with SOC and without SOC effects.

References

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