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Coupled Exciton - Surface Plasmon Polariton Enhanced Photoresponse of Two-Dimensional Hydrogenated Honeycomb Silicon Boride

Authors : Farzaneh Shayeganfar, Ali Ramazani

Abstract : Exciton (strong electronic interaction of electron-hole) and hot carriers created by surface plasmon polaritons has been demonstrated in nanoscale optoelectronic devices, enhancing the photoresponse of the system. Herein, we employ a quantum framework to consider coupled exciton- hot carriers effects on photovoltaiv energy distribution, scattering process, polarizability and light emission of 2D-semicnductor. We use density functional theory (DFT) to design computationally a semi-functionalized 2D honeycomb silicon boride (SiB) monolayer with H atoms, suitable for photovoltaics. The dynamical stability, electronic and optical properties of SiB and semi-hydrogenated SiB structures were investigated utilizing the Tran-Blaha modified Becke-Johnson (TB-mBJ) potential. The calculated phonon dispersion shows that while an unhydrogenated SiB monolayer is dynamically unstable, surface semi-hydrogenation improves the stability of the structure and leads to a transition from metallic to semiconducting conductivity with a direct band gap of about 1.57 eV, appropriate for photovoltaic applications. The optical conductivity of this H-SiB structure, determined using the random phase approximation (RPA), shows that light adsorption should begin at the boundary of the visible range of light. Additionally, due to hydrogenation, the reflectivity spectrum declines sharply with respect to the unhydrogenated reflectivity spectrum in the IR and visible ranges of light. The energy band gap remains direct, increasing from 0.9 to 1.8 eV, upon increasing the strain from -6% (compressive) to +6% (tensile). Additionally, compressive and tensile strains lead, respectively, to red and blue shifts of optical the conductivity threshold around the visible range of light. Overall, this study suggests that H-SiB monolayers are suitable as two-dimensional solar cell materials.

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