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Investigating the electro-optical properties of 3D superlattices and 2D materials: A DFT study

The electromagnetic radiations can propagate in space, which could interact with the matter in various ways. Advancement in the electronic industry demands to explore new materials with pronounce electronic and optical features. Due to the boosted semiconductor industry, the optoelectronic devices are extensively employed in manufacture, medicine, astronomy, automobile, communications, military, and so on, reshaping our lives. These include light emitting diodes, semiconducting lasers, photovoltaic devices, photodiodes and photodetectors. Previous studies incorporate the investigation of optoelectronic properties for different materials such bulk systems, alloys, thin films and 2D layered structures. Currently, the Ga- and Hg-free type-II superlattices of InAs/(InAsSb) are highly demanding in the infrared industry due to their unique optoelectronic properties. Moreover, the distinct mechanical and electro-optical features of the newly discovered 2D materials family MA_2Z_4 as compared to other 2D materials necessitates further studies to explore this 2D material class.

Motivated from the outstanding characteristics of Ga- and Hg-free type-II superlattices of InAs/(InAsSb), and the extraordinary mechanical and electro-optical features of MA_2Z_4 family, we explore here the electronic and optical properties of $InAs/InAs_{0.625}Sb_{0.375}$ 3D superlattice (SL), 2D materials XSi_2N_4 (X = Mo, W, and Ti) and their vertical/lateral heterostructures $MoSi_2N_4/XSi_2N_4$ (W, Ti), and Janus structures.

In the study of $InAs/InAs_{0.625}Sb_{0.375}$ 3D superlattice, the modified Becke-Johnson exchange-correlation functional is employed to have a good description of the electronic and optical properties. The bulk InAs and InSb are analyzed first and then the $InAs/InAs_{0.625}Sb_{0.375}$ superlattice for the three lattice constants of the bulk InAs, GaSb and AlSb is investigated, respectively. A strong dependence of electronic and optical properties on the variation of lattice constant is observed. There exists two heavy-hole bands with increasing in-plane effective mass as one goes far from the Fermi level. In addition, a considerable decrease in the effective masses for heavy-holes and energy gaps in the k_x-k_y plane is noticed as compared to their bulk phases of the parent compounds. We noticed that the electrons are delocalized in the InAs part of SL, while the holes mainly are localized in the $InAs_{0.625}Sb_{0.375}$ part. The absorption spectra in the far-infrared regime are strongly increased in the case of the aforementioned superlattice with respect to bulk InAs and InSb suggesting their applications in long-wavelength IR detectors.

In the second project, we discuss newly discovered 2D layered materials such as XSi_2N_4 (X = Mo, W, and Ti), and their vertical and laterally stitched 2D heterostructures $MoSi_2N_4/XSi_2N_4$ (X=W, Ti). We report that all the systems are structurally stable as confirmed by the total energy ground state calculations and the phonon spectra. After establishing their thermodynamical stability, we study the electronic band structures and the density of states of the monolayers XSi_2N_4 (X = Mo, W, and Ti) and 2D heterostructures, respectively. Both the monolayers and the heterostructures demonstrate a semiconducting behavior with band gaps ranging from the infrared to the visible region. From the electronic band structures, we noticed that the band gap of $MoSi_2N_4/WSi_2N_4$ lies in the visible region employing their applications for photovoltaics and other optoelectronic devices. Instead, in the $MoSi_2N_4/TiSi_2N_4$ wherein the 'W' is replaced with 'Ti', the band gap drops to the IR range, thus providing the possibility to utilize these heterostructures as IR detector materials. In the third project, we extend the study of laterally stitched 2D heterostructures to investigate the effect of biaxial strain on the electronic and optical properties, which reveals significant modifications in the electronic band structures and optical spectra. We observed a transition from indirect to direct band gap semiconductor with the compressive strain in $MoSi_2N_4/WSi_2N_4$. Similarly, the biaxial strain causes a semiconducting to metallic transition in $MoSi_2N_4/TiSi_2N_4$. Besides, the optical spectra including absorbance, transmittance and reflectance can be tuned effectively using strain engineering. Our findings based on the electro-optical properties and their controlled modulation via biaxial strain suggest that these newly discovered 2D materials and heterostructures could be useful in nano- and optoelectronics.

Lastly, we study the pristine $MoSi_2P_4$ and Janus phase $XGeSiP_2As_2$ (Mo, W) in this new family of 2D materials. The appearance of high cohesive energies and the absence of imaginary phonon modes confirm their stability and possible experimental realization. The Janus structures indicate small direct band gaps and larger spin splittings at K/K' in comparison to pristine $MoSi_2P_4$. The monolayered structure of Janus material possesses the broken mirror symmetry that gives rise to a potential gradient, which is normal to the plane of the material. This generates a difference in the work function of 2D material for the two surfaces. In addition, it is exposed from the spin textures that the broken mirror symmetry causes the Rashba spin-splitting in the Janus monolayers, which can be increased by using higher atomic spin-orbit coupling. In the supplementary material, we manifest and compare the optical spectra for pristine and Janus phases revealing characteristic absorption peaks in the infrared region. The large spin and Rashba-type splittings together with the exceptional optical spectra in the Janus structures can make an extraordinary contribution to the valleytronics, spintronics and IR applications.

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