

A.11: Direct band gaps in Phosphorene-like Group IV-VI monolayers

Search of novel monolayer materials is one of the important goals of material science and condensed matter physics research activities. After the discovery of graphene, several two-dimensional (2D) monolayered materials have been theoretically predicted and then synthesized experimentally. Until now, the following 2D monolayers have been successfully synthesized by various experimental groups all over the world: in group III Borophene; in group IV Silicene, Germanene, Stanene; in group V Phosphorene. In our group, we have predicted the stability and properties of 2D materials aluminene, arsenene, silicene multilayers and their hybrid structures. Recently, multilayers of silicene and arsenene have been synthesized and their properties are being studied by various experimental techniques. Though graphene possesses many interesting novel properties, the major disadvantage with graphene is that it has no electronic band gap and hence it is difficult to use graphene for semiconductor device applications. Recently, phosphorene, a monolayer of phosphorus, has attracted much attention of the researchers since it has an appropriate band gap for electronics applications and is shown to act as a field-effect transistor.

In order to search for phosphorene like alternate 2D materials, we have performed systematic investigations on the geometric, energetic, and electronic properties of group IV-VI binary monolayers (XY) by employing density functional theory based electronic structure calculations. For this purpose, we choose the binary systems XY consisting of equal numbers of group IV ($X = C, Si, Ge, Sn$) and group VI elements ($Y = O, S, Se, Te$) in three geometrical configurations - the puckered, buckled and planar structures. The results of binding energy calculations (See Fig. A.11.1 (a)) show that all the binary systems studied are energetically stable. It is observed that the puckered structure, similar to that of phosphorene, is the energetically most stable geometric configuration. Moreover, the binding energies of buckled configuration are very close to those of the puckered configuration. Our results of electronic band structure predict that puckered SiO and CSe are direct band semiconductors with gaps of 1.449 and 0.905 eV, respectively (See Fig. A.11.1 (b) and (c)). Band structure of CSe closely resembles that of phosphorene. Remaining group IV-VI binary monolayers in the puckered configuration and all the buckled monolayers are also semiconductors, but with indirect band gaps. Importantly, we find that the difference between indirect and

direct band gaps is very small for many puckered monolayers. Thus there is a possibility of making these systems undergo transition from indirect to direct band gap semiconducting state by a suitable external influence. Indeed, we show in the present work that seven binary monolayers, namely, SnS, SiSe, GeSe, SnSe, SiTe, GeTe and SnTe become direct band gap semiconductors when they are subjected to a small mechanical strain ($\approx 3\%$).

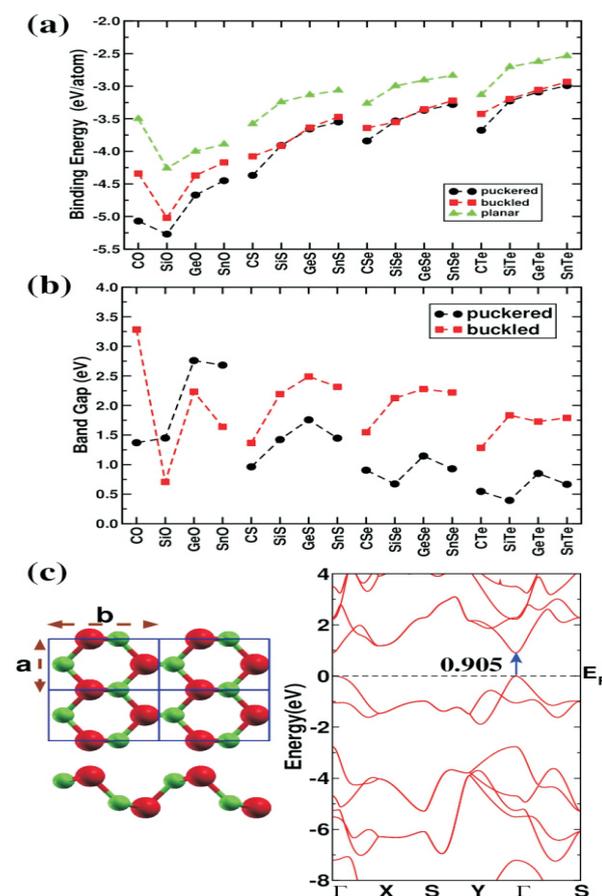


Fig. A.11.1: (a) Binding energy and Band gaps for group IV-VI monolayers. (b) Band structure of puckered CSe. (c) Optimized geometric structures (top & side views) and band structure of puckered CSe.

This makes nine out of sixteen binary monolayers studied in the present work direct band gap semiconductors. Thus there is a possibility of utilizing these binary counterparts of phosphorene in future light-emitting diodes and solar cells. [For more details, please refer to C. Kamal et al, Phys. Rev. B 93, 125428 (2016)] .

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