Should we expect graphitic structures among the binary semiconductors?

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Ionic semiconductors such as ZnO which have a wurtzite crystal structure favoured in the bulk are known to favour graphitic structures in the ultrathin limit to avoid a polar catastrophe[1]. In this work, we consider the more covalent examples of II-VI and III-V semiconductors and examine if a graphitic phase can be realized in these cases. In the graphitic limit going from bulk to the monolayer, the coordination number decreases. As a result, the bond length decreases to make up for the lost bandwidth. However, moving away from elements of the first row of the periodic table, one finds that the wavefunctions associated with the valence electrons are more extended. As a result of this, the coulomb interaction between the electrons on the cation and anion increases. The system responds by going to a buckled structure, elongating the anion-cation bond[2,3]. This buckled structure has a dipole moment associated with it which is of tremendous interest because of their potential valley-dependent properties. The loss of inversion symmetry in these structures also results in the coupling of spin and valley physics[4]. Examining the phonon dispersion of these materials, we find a soft mode at the zone boundary. Allowing for displacements according to the forces associated with the soft mode, one finds a ground state structure with no dipole moment.

References

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