

New structures for two-dimensional III-V binary compounds

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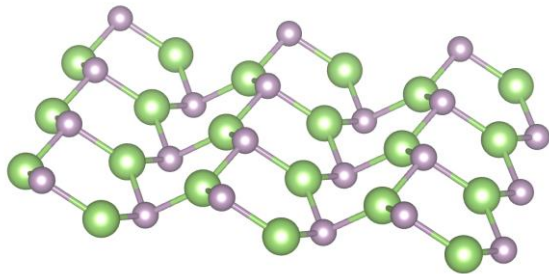
Using first-principles calculations, we propose new two-dimensional structures for III-V binary compounds that are energetically more favorable than the theoretical structures that have been proposed so far [1,2]. These new 2D crystals show interesting mixtures of sp^2 -hybridized cations and sp^3 -hybridized anions. Their formation energies are substantially lower (up to 300 meV/atom) than the planar graphene-like and low-buckled silicene-like counterparts and are comparable to the rectangular structures proposed by Zhuang *et al.* [2]. The origin of the high stability of our proposed structures is twofold: (i) in contrast to the low-buckled structures, the proposed structures have no electric dipole that destabilizes the system and (ii) our structures have favorable orbital hybridizations for the cations and anions. It is well-known from molecular chemistry that group-III elements prefer planar sp^2 -bonded structures as in trihydrides and trihalides. Group-V elements, on the other hand, prefer tetragonal sp^3 -bonded configurations. We found two stable configurations with these favorable hybridizations (see figure) and investigated their properties with *ab initio* calculations.

References

- [1] H. Sahin, S. Cahangirov, M. Topsakal, E. Bekaroglu, E. Akturk, R. T. Senger, and S. Ciraci, *Phys. Rev. B*, **80** (2009) 155453.
[2] H. L. Zhuang, A. K. Singh, and R. G. Hennig, *Phys. Rev. B*, **87** (2013) 165415.

Figures

(a)



(b)

