Computational synthesis of single-layer III-V materials

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Graphene has been of great interest since its discovery in 2005. The importance of graphene is not only that it has unique properties but also that it has promoted the interest in the isolation and synthesis of other 2-D materials, e.g. BN, MoS2, ZnO, NbSe2, with a variety of interesting properties, from insulators to metal, from mechanically strong to soft, and chemically active to chemically inert. In our recent work [1], using a first principles design approach, we have identified a previously unrecognized large family of mono layer group III-V materials. Three different structures that are energetically and dynamically stable in various materials of this family have been identified, namely a planar honeycomb hexagonal structure, a buckled hexagonal structure, and a surprising low-energy tetragonal structure. In this poster we show, using density functional theory, a synthesis approach for these as-yet hypothetical novel 2-D materials. We have identified several lattice-matched and symmetry-matched metallic substrates for the synthesis of these 2-D materials. These substrates stabilize the 2-D III-V materials by reducing the formation energies of the 2-D materials in comparison to their bulk counterparts. The 2-D III-V materials range from semiconductors to metals and from mechanically stiff to very soft. The predicted suitable substrates enable the tuning of the electronic properties of these 2-D materials. Our results provide guidance for experimental synthesis and an engineering methodology for the electronic properties of these novel 2-D III-V materials.

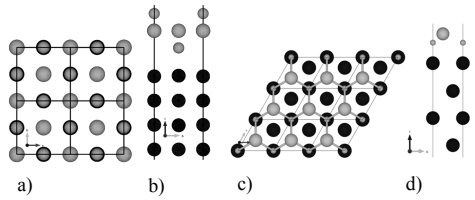

Figure 1: a-b) Top & side view of 2-D tetragonal AlP adsorbed on Pd (100) surface. c-d) Top & side view of 2-D hexagonal InN adsorbed on Ho (111) surface.

[1] H. L. Zhuang, A. K. Singh, and R. G. Hennig, Computational discovery of single-layer III-V materials, Phys. Rev. B, 87, 165415 (2013).