Single-layer boron phosphide on metallic surfaces: screening of promising substrates by first-principles

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Single-layer hexagonal boron phosphide (hBP) is a predicted honeycomb-structured semiconductor exhibiting interesting properties for photovoltaic and photocatalytic applications [1] and is the most stable [2] between its proposed allotropes [3]. We investigate by ab-initio calculations the ground-state properties of hBP on FFC (111) surfaces of different d-shell metals, with the aim of identifying suitable substrates for its synthesis. Due to the lattice parameter mismatch with the substrates, the hBP overlayer generates Moiré patterns that we describe using minimal simulation cells (Figure 1a) with a tolerance of 3% for tensile or compressive strain applied to the overlayer. Adhesion energy, average overlayer-substrate distance (Figure 1b), charge transfer, projected density of states indicate that the least(most) interacting substrate is Ag(Au), with the smallest(largest) buckling, which is patterned by the substrate (Figure 1c).
We complete the investigation of hBP on Ag (111), which is therefore the ideal candidate for hBP growth, by also examining its atom-by-atom growth process, influenced by the competition between phosphorus and boron attachment at the edges of the already formed islands.

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References

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Figures

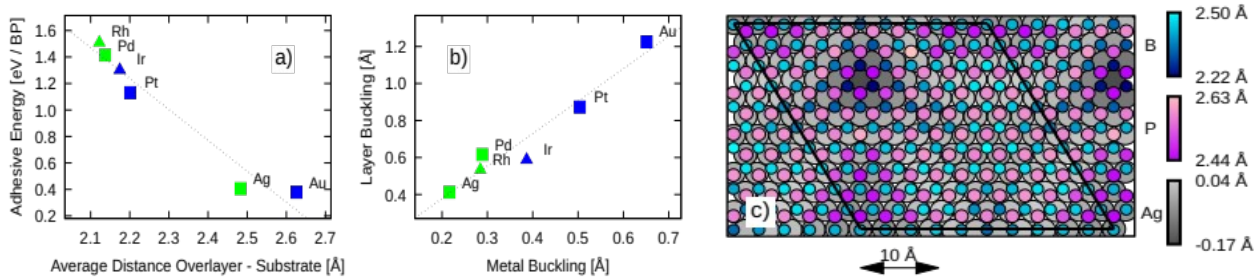

Figure 1: a) Adhesive energy of hBP over selected transition metal substrates (Rh, Pd, Ag, Ir, Pt, Au) with respect to the average BP-substrate distance. b) Buckling of hBP overlayer with respect to that of the substrate surface atoms. In a) and b), dashed lines are a guide to the eye. c) Optimized model for the Moiré pattern of hBP over Ag(111) with the sketch of the simulation cell; the colour scale indicates the individual height of the overlayer and surface atoms.