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First-principles investigation of the electronic structure of the α-Al2O3-graphene interface

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Abstract

First-principles calculations reported here illuminate the effects of the interface properties of Al_2O_3 and graphene, with emphasis on the structural and electrical properties. Various contact interfaces and with different alpha-Al_2O_3 surface terminations are considered with on and slightly-off stoichiometric aluminum oxide. We show that depending on whether aluminum or oxygen is near graphene, a sp^3 structural deformation and spontaneous spin-polarization may occur next to the interface contact [1,2] (see Fig. 1). Interestingly, when the oxygen atoms near graphene do not cause such deformation, and for specific stoichiometries of the alumina layer, the Dirac cone of the graphene band structure shifts to lie above the Fermi level. This Such shifts suggest p-type doping, which primarily has its origin from the oxygen atoms, for situations when hybridization between O and the graphene is weak. We also show that our analysis supports the observation done in recent experiments [3]

References

[1] Y. Feng, D. J. Trainer, and K. Chen, Applied Physics, 164505 (2016).
[2] T. French and G. A. Somorjai, Physical Chemistry, 2489 (1970).
[3] Belotcerkovtceva, Daria; Maciel, Renan P. et al; ACS Applied Materials & Interfaces, (2022)

Figures

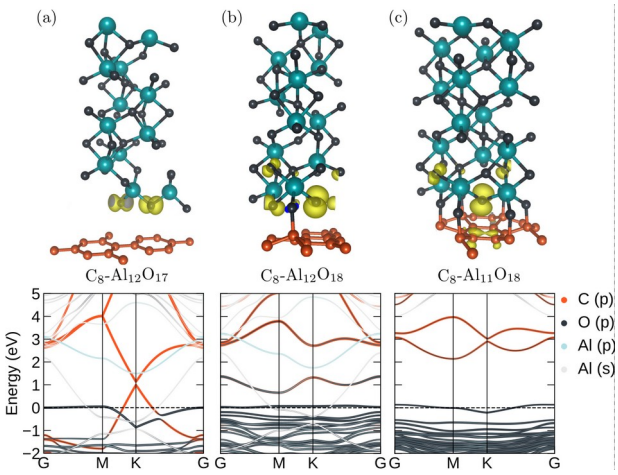

Figure 1: Alumina-graphene interface and its respective band structures. (a) shows the structure as well as the band structure when alumina presents (a) an oxygen deficiency, (b) no deficiency, and (c) an aluminum deficiency.