First-Principles Simulations of Graphene Hybrid Structures

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The design of graphene heterostructures is a research field of rising importance. It is nowadays possible to combine graphene with other layered 2D materials which offers promising possibilities for novel nanodevices[1]. Here, we present first-principles simulations of interfaces between graphene and other layered 2D materials, such as boron nitride[2] or the transition metal dichalcogenide MoS2. We discuss electronic and structural properties of the hybrids and compare the results to experiments.

[1] K. S. Novoselov, V. I. Fal'ko, L. Colombo, P. R. Gellert, M. G. Schwab & K. Kim, *Nature* **490**, 192 (2012).
[2] B. Sachs, T. O. Wehling, M. I. Katsnelson & A. I. Lichtenstein, *Phys. Rev. B* **84**, 195414 (2011).