Transferable Tight-Binding Models for Graphene/hBN Heterostructures

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We present an effective tight-binding model for graphene/hexagonal boron nitride (hBN) heterostructures that accurately captures the influence of the hBN substrate on the electronic structure of graphene. The model is parametrized using *ab initio* data from density functional theory (DFT) calculations of untwisted, lattice-matched graphene–hBN systems, thereby avoiding the need for large moiré supercells. Despite this minimal training set, the model generalizes well to realistic configurations with twist angles, lattice mismatch, and structural relaxation. It is applicable to both monolayer and bilayer graphene, whether deposited on or fully encapsulated by hBN. Unlike previous models [1,2], our approach naturally incorporates relaxation effects, making it compatible with classical force-field-based structural relaxation. Furthermore, in contrast to Slater–Koster-based approaches [3], our Hamiltonian includes only graphene degrees of freedom, with the influence of hBN captured effectively—eliminating the need to explicitly specify the form of the graphene–hBN coupling. This approach provides a computationally efficient and transferable framework for moiré materials and engineered van der Waals heterostructures.

References

[1] P. Moon, M. Koshino, Phys. Rev. B 90, 155406 (2014)
[2] M. Kindermann, B. Uchoa, D. L. Miller, Phys. Rev. B 86, 115415 (2012)
[3] M. Long, et al., Phys. Rev. B 107, 115140 (2023)

Figures

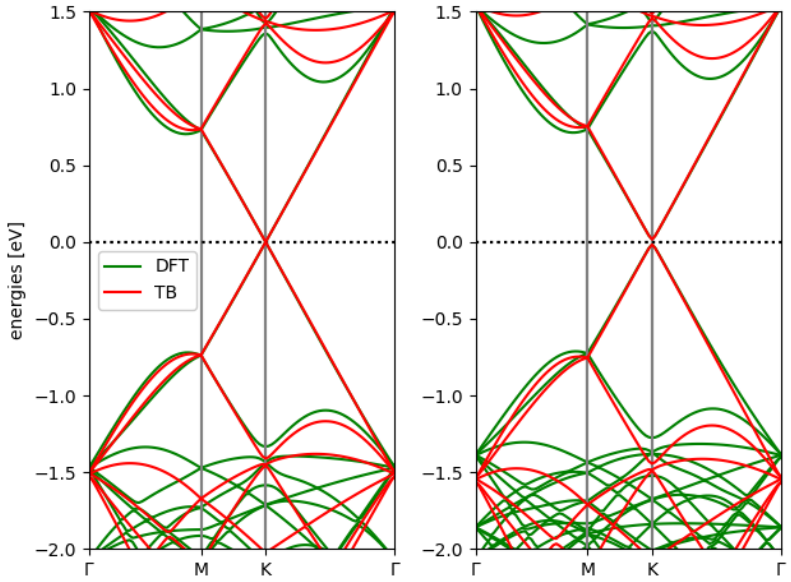

Figure 1: DFT (green) and effective TB model (red) band structures for twisted monolayer graphene on hBN (left), and twisted encapsulated hBN-graphene/hBN (right) for a 9.4° twist.