Multiscale model of adhesion and strain in graphene on hexagonal boron nitride

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Double-layer devices based on single layer graphene-on-hBN (SLG/hBN) are of great interest for electronic and optical applications. We present calculations of the binding energy (BE) of SLG/hBN for four configurations shown in Fig.1 using variational and diffusion quantum Monte Carlo (DMC) calculations as implemented in the CASINO code [1]. We evaluate the DMC BE as functions of local lattice mismatch, which may serve as benchmarks or the development of more approximate first-principles methods, such as density functional theory with dispersion corrections. Our DMC results in Fig.2 are used to parametrise an adhesion potential as a function of local lattice offset between hBN and SLG. Using a continuum model of the elastic energy and the adhesion potential [2,3] as a function of the continuous displacement field of the hBN layer, we find a unique solution for the displacement field at each small misalignment angle. This implies that observed differences in the properties of exfoliated graphene transferred onto hBN and graphene directly grown on hBN may be due to differences in type and concentration of defects rather than the structure of the G/hBN bilayer itself.

References

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[2] San-Jose, et al., Phys. Rev. B 90, 075428 (2014)
[3] Aitken, Huang, J. Appl. Phys. 107, 123531 (2010).

Figures

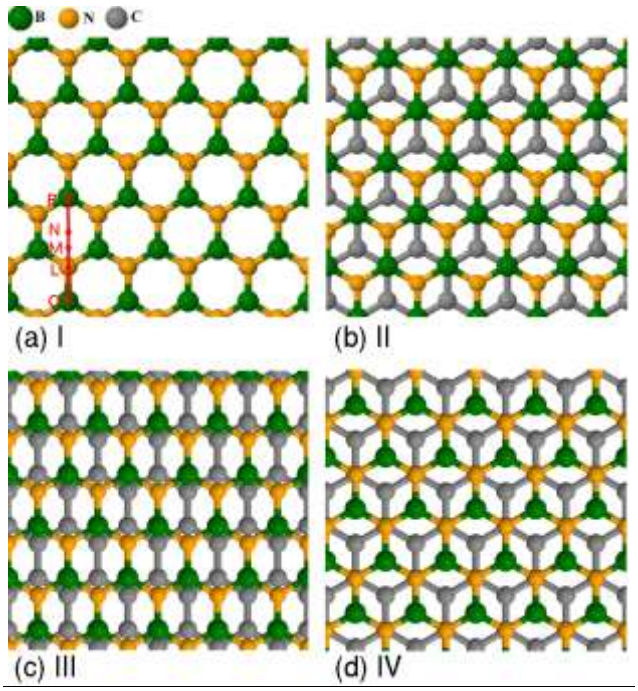

Figure 1: SLG/hBN stacking configurations considered in our work.

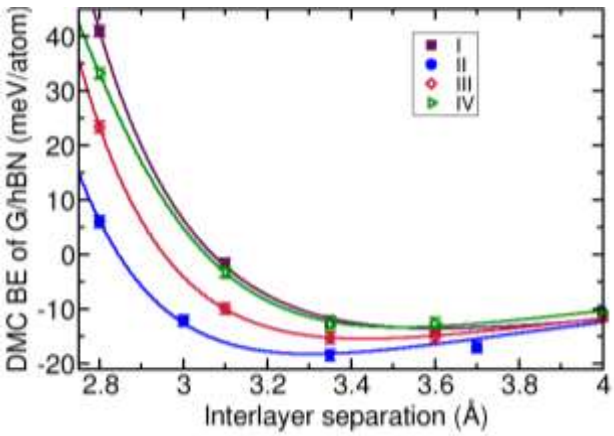

Figure 2: DMC BE of SLG/hBN as a function of interlayer separation