

Abstract Submitted  
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**Spatial dependent van der Waals energy between graphene and boron-nitride** MEHDI NEEK-AMAL, FRANCOIS PEETERS, Departement Fysica, Universiteit Antwerpen, CONDENSED MATTER GROUP, UNIVERSITY OF ANTWERP COLLABORATION — The small mismatch between the honeycomb lattices of graphene (GE) and boron nitrate (h-BN) leads to long wavelength Moiré patterns. In order to describe such patterns it will require large size unit cells that are unattainable with *ab-initio* calculations. Earlier density functional theory calculations imposed lattice matching between graphene and h-BN which induces strain and opens a gap of 4 meV [1]. In previous works the Moiré pattern in GE/h-BN was connected to the van der Waals interaction [2], but a clear theoretical microscopic analysis is still missing. We used atomistic simulations [3] with very large unit cells to investigate quantitative aspects of the connection between the vdW interaction and the Moiré patterns. The value and symmetry of the spatial dependent vdW energy is obtained which agrees with the recently reported Moiré patterns. *Acknowledgement:* This work was supported by FWO-VI, EU-Marie Curie and the Methusalem foundation. [1] B. Sachs *et al*, Phys. Rev. B **84**, 195414 (2011); M. Zarenia *et al*, Phys. Rev. B **86**, 085451 (2012). [2] C.R. Dean *et al*, Nat. Nanotech. **5**, 722 (2010); J.H. Chen *et al*, Nat. Nanotech. **3**, 206 (2008). [3] M. Neek-Amal and A. Lajevardipour, Comp. Mat. Sc. **49**, 839 (2010).

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