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Comparison of methods for inclusion of van der Waals interactions: the case of physisorption of nucleobases on graphene[1] DUY LE, ABDELKADER KARA, TALAT S. RAHMAN, University of Central Florida — The physisorption of the nucleobases adenine (A), cytosine (C), guanine (G), thymine (T), and uracil (U) on graphene is studied using many flavors of density functional theory (DFT): the generalized gradient approximation (GGA) with the inclusion of van der Waals (vdW) interaction based on the TS approach [A. Tkatchenko and M. Scheffler, *PRL* **102**, 073005 (2009)], our simplified version of this approach, the vdW density functional (vdW-DF) [M. Dion *et al.*, *PRL* **92**, 246401 (2004)], and the vdW-DF2 [K. Lee *et al., PRB* **82**, 081101 (2010)] methods. The binding energies of nucleobases on graphene lie in the range of 496962 meV and are found to be in the following order G>A>T>C>U within vdW-DF, vdW-DF2 and our method and G>A>T∼C>U in the TS approach. The binding separations lie between 3.293.53 Å and are found to be about 0.1 0.2 Å shorter in DFT-D, as compared to vdW-DF approaches. We comment on the efficiency of combining the DFT-D and vdW-DF methods to study vdW interactions in molecular adsorption.

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