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Physisorption of nucleobases on graphene: the role of van der Waals interactions[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 within the generalized gradient approximation (GGA) of the density functional theory (DFT) with the inclusion of van der Waals interaction (vdW) based on the London dispersion equation. We find that the inclusion of the latter interaction increases the binding energy by about 0.5eV (from an almost zero value) and moves these nucleobases by about 0.5Å toward the graphene, as compared to the results obtained with regular DFT-GGA. The binding energies of nucleobases on graphene are found to be in the following order: G>A>T>C>U, with a dispersion of about 200meV. Details of the dynamics (diffusion barriers) and adsorption characteristics of these nucleobases on graphene will be presented as well as the description of their electronic structure and nature of the bonding with the substrate.

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