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Diffusion Monte Carlo ab initio calculations to study wetting properties of graphene YANBIN WU, HUIHUO ZHENG, LUCAS WAGNER, N.R. ALURU, University of Illinois — For applications of graphene in water, including for example desalination and DNA sequencing, it is critical to understand the wetting properties of graphene. In this work, we investigate the wetting properties using data from highly accurate diffusion quantum Monte Carlo (DMC) calculations, which treat electron correlation explicitly. Our DMC data show a strong graphene-water interaction, indicating graphene surface is more hydrophilic than previously believed. This has been recently confirmed by experiments [Li et al. Nat. Mater. 2013, doi:10.1038/nmat3709]. The unusually strong interaction can be attributed to weak bonding formed between graphene and water. Besides its inadequate description of dispersion interactions as commonly reported in the literature, density function theory (DFT) fails to describe the correct charge transfer, which leads to an underestimate of graphene-water binding energy. Our DMC calculations can provide insight to experimentalists seeking to understand water-graphene interfaces and to theorists improving DFT for weakly bound systems.

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