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Developing of van der Waals parameters for graphitic carbon-water interaction using ab initio methods YANBIN WU, NARAYANA ALURU, University of Illinois — In this study, graphitic carbon-water van der Waals interaction parameters are developed entirely from first-principle calculation data. First, the Møller-Plesset perturbation theory of the 2nd order (MP2) method is employed to compute the polycyclic aromatic hydrocarbon-water interaction energies. The proper size of basis sets is utilized in the MP2 calculations and the energy component analysis is performed to extrapolate to infinite-sized graphene limit. Then, graphitic carbon-water interaction parameters are developed based on the MP2 results from this work and the ab initio data available in the literature from other methods such as random-phase approximation (RPA), diffusion Monte Carlo (DMC), density functional theory-symmetry-adapted perturbation theory (DFT-SAPT) and couple cluster treatment with single and double excitations and perturbative triples (CCSD(T)). We evaluate the accuracy of the interaction parameters by predicting water contact angle on graphite and compare it with experimental data. The interaction parameters based on RPA, DFT-SAPT and corrected DMC data predict contact angles which agree well with experiments, while the parameters based on MP2 and CCSD(T) data have the tendency to underestimate the contact angle.

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