A simple potential for graphene-fluid interactions

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A simple analytical potential function for calculating the interaction between a fluid molecule and a graphene sheet was developed and examined in simulations. The dispersion/repulsion, induction, dipole-quadrupole, quadrupole-quadrupole interactions between a fluid particle and a single layer of graphene sheet are described by integrated functions that are only dependent on the separation between the fluid molecule and the graphene along the graphene surface normal. The derived potential functions are in excellent agreement with the computationally demanding atom-explicit summation method. Typical errors of the integrated potential are less than 2\% in the potential well minimum compared with the exact atom-explicit summation. Monte Carlo simulations were performed to model the adsorption of two representative gases in graphene sheets using both the integrated potential and atom-explicit potential. The integrated potential results in the same adsorption isotherms and density profiles for the adsorbed phase compared with the atom-explicit summations while the computational time for the simple potential is negligible compared with that using the atom-explicit summations. The derived potentials provide a convenient approach that can be used in calculating the physical interaction between fluids and graphene sheets.