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Hexagonal Boron Nitride-Water Non-bonded Interaction from First Principles YANBIN WU, LUCAS K. WAGNER, NARAYANA R. ALURU, Univ of Illinois - Urbana — The interaction between water and h-BN is estimated using the Møller-Plesset perturbation theory of the second order (MP2) and diffusion Monte Carlo (DMC) method. The MP2 and DMC results are verified using coupled cluster treatment with single and double excitations and perturbative triples at the complete basis set limit (CCSD(T)/CBS) using B3N3H6-water as a proxy. The water-h-BN binding energy is estimated as 1.9 $\pm$ 0.2 kcal/mol. Boron/nitride (BN)-water non-bonded interaction parameters are developed based on the MP2 energies. The B/N-water parameters predict the water contact angle on bulk h-BN surface that is in good agreement with experimental measurements.

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