

The Quantum Monte Carlo studies of interactions in van der Waals bilayer systems

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The van der Waals (vdW) interaction is one of the most fundamental physical quantities resulting from quantum fluctuation of charges. However, it remains a challenge to account for this interaction quantitatively in both theory and experiment. In recent years, there have been many proposed vdW functionals attempted to overcome this deficiency; however, discrepancies in the obtained binding energies using different vdW functionals are usually apparent.

In this work, we present the results of the binding energy for various two-dimensional (2D) bilayer systems: BN/BN [1], Silicene/BN, Silicene/Graphene, and MoS₂/Graphene using Diffusion Monte Carlo (DMC) and density functional theory (DFT) with LDA, GGA, and various vdW functionals. The DMC results of binding energy and the behavior beyond the equilibrium distance have diverse differences from those obtained by DFT with LDA, GGA, and vdW functionals. The outcome of present study would serve as the benchmark of 2D bilayer systems for various DFT vdW functionals and guidance for prospective experiments.

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[1] C. R. Hsing, C. Cheng, J. P. Chou, C. M. Chang, C. M. Wei, *Van der Waals interaction in a boron nitride bilayer*, New Journal of Physics, 16, 113015 (2014)