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(POS-29) Many-Body Dispersion in Model Systems and the Sensitivity of Self-Consistent Screening

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London dispersion is a weak, attractive, intermolecular force that occurs due to interactions between instantaneous dipole moments. While individual dispersion contributions are small, they are the dominating attractive force between non-polar species and determine many properties of interest. Standard methods in density-functional theory do not account for dispersion contributions, so a correction such as the exchange-hole dipole moment (XDM) or many-body dispersion (MBD) models must be added. Recent literature has discussed the importance of many-body effects on dispersion, and attention has turned to which methods accurately capture them. By studying systems of interacting quantum harmonic oscillators from first principles, we directly compare computed dispersion coefficients and energies from XDM and MBD. While the results are similar at large separations, MBD is found to be susceptible to a polarization catastrophe at short range. Additionally, the self-consistent screening formalism used in MBD is shown to be surprisingly sensitive to the choice of input polarizabilities. Connection is made to interactions between noble gas atoms, as well as to the methane and benzene dimers, and to two layered materials, graphite and MoS2, for which similar results to the oscillator models were obtained.

Keyword-1

Density-Functional Theory

Keyword-2

London Dispersion

Keyword-3

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