Application of Diffusion Monte Carlo to Materials Dominated by van der Waals Interactions.

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van der Waals forces are notoriously difficult to account for from first principles. We have performed extensive calculations to assess the usefulness and validity of diffusion quantum Monte Carlo when predicting van der Waals forces. We present converged results for noble gas solids and clusters, archetypical van der Waals dominated systems, as well as the highly relevant π-π stacking supramolecular complex: DNA + intercalating anticancer drug ellipticine. Analysis of the calculated binding energies underscores the existence of significant interatomic many-body contributions.
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