

Course Graining Fermions: Accurate Helium Clusters via Tensor Product State Representations

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Helium clusters are interesting for their applications in ultracold chemistry reaction chambers and spectroscopy medium, but are weakly bound and unstable making them extremely difficult to study. We use tensor product selected configuration interaction (TPSCI) as a computationally efficient approach that reaches near full CI results to study these helium atom clusters. TPSCI allows the use of large basis set representation for various calculations like ground state and excited state energies. Additionally, we are able to directly measure the role of many-body dispersion in the binding energy.