Quantum Embedding Using the Huzinaga Level-Shift Projection Operator for Complex Systems

Scientific Achievement

A wave-function (WF) in density functional theory (DFT) embedding method using the Huzinaga level-shift projection operator was studied for its accuracy compared to full WF methods. The energies of a diverse set of complex systems were computed with the projection operator and consistently converged with the intensive full WF results.

Significance and Impact

Full WF methods are computationally demanding and expensive: the Huzinaga embedding scheme is efficient and robust for large and complex systems, as demonstrated with the Fe-MOF-74 cluster model.

Research Details

Using the Huzinaga level-shift projection operator in a WF-in-DFT embedding method proved accurate and efficient across diverse systems.

- The systems include partitioning across two covalent bonds and a conjugated π network and gas adsorption onto transition metals.
- The embedding method developed here is applicable to much larger, beyond current WF level calculations.

The Huzinaga level-shift projection operator with WF-in-DFT method was used to calculate the H₂ adsorption energies of the complex Fe-MOF-74. The performance of the new method is comparable within 2 kcal/mol to the full-system CASPT2-in-M06 results.