

Non-additive intermolecular interactions, involving three or more molecules, present a significant challenge in accurately predicting molecular behaviour and properties of materials. These interactions, characterized by their high-dimensional and unpredictable nature with molecular position, cannot be reliably estimated by simply summing pairwise interactions between molecules. Incorporating three-body non-additive interactions into first-principles quantum mechanical approaches can greatly enhance agreement with experimental data, often achieving remarkable reductions in deviations.