
Noncovalent interactions: Making calculations more accurate and more insightful

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Accurate intermolecular interaction energies are indispensable as data points for potential energy surfaces and as benchmark values for improving and testing more approximate approaches. The gold standard for computing these energies is the supermolecular coupled-cluster method with singles, doubles, and perturbative triples (CCSD(T)) converged to the complete basis set (CBS) limit, which normally requires performing CCSD(T) in a basis set of at least triple-zeta quality. When a triple-zeta CCSD(T) calculation is not feasible but a double-zeta one is, it is worthwhile to look for a silver standard that provides the most accurate and consistent approximation to the gold standard at a reduced computational cost. A common disadvantage of all supermolecular standards is that they give a single number that says nothing about the nature of interaction. A successful alternative is provided by symmetry-adapted perturbation theory (SAPT), where the interaction energy is computed as a sum of physically distinct electrostatic, exchange, induction, and dispersion contributions. The recent studies from our group aim at:

1. increasing the capabilities of SAPT, targeting spin splittings, basis set convergence, and intramolecular interactions,
2. establishing the best strategies for computing silver-standard CCSD(T)/CBS estimates through explicit correlation and midbond functions, and
3. applying accurate supermolecular and SAPT approaches to gain novel insights into the interaction in chemically important complexes.