# Predictions for water clusters from a first-principles two- and three-body force field

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We present [1] a new rigid-monomer three-body potential for water obtained by fitting over 70 thousand three-body non-additive energies computed using coupled-cluster method with singles, doubles and non-iterative triples [CCSD(T)] with augmented triple-zeta-quality basis sets. The potential is used in conjunction with a modified version of the two-body CC-pol-5s and CC-pol-8s series of potentials that provided successful predictions for wide range properties of water [2–4]. This new potential is used with a newly-developed polarization model for four- and higher-body interactions to compute energies of the water trimers, hexamers and 24-mers. The new potential denoted as CCpol23+ improves the interaction energies compared to the former CC-pol potentials and despite using the rigid-monomer approximation, provides predictions as accurate or better with respect to flexible-monomer benchmarks compared to published flexible-monomer force fields. We also show that, surprisingly, our polarization model can predict four-body interaction energy to within a few percent, even though polarization models for three-body interactions have errors of the order of 50%.

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