# An automated Calculation Pipeline for Differential Pair Interaction Energies with Molecular Force Fields using the Tinker Molecular Modeling Package

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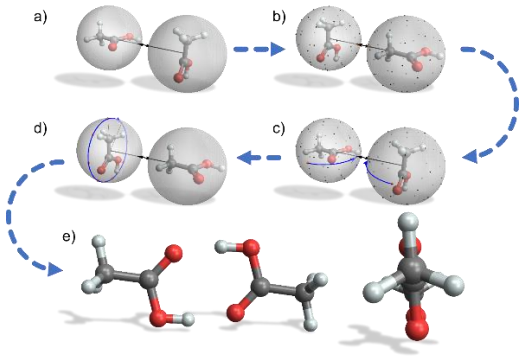
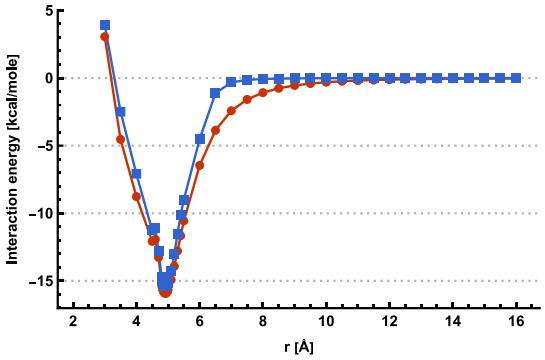
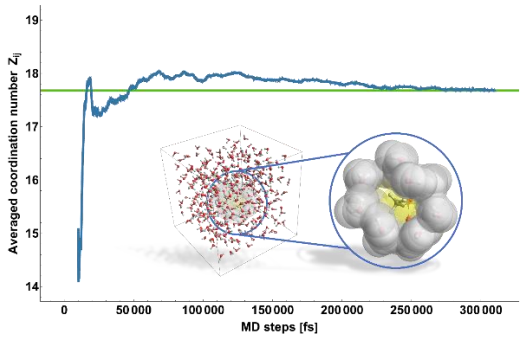
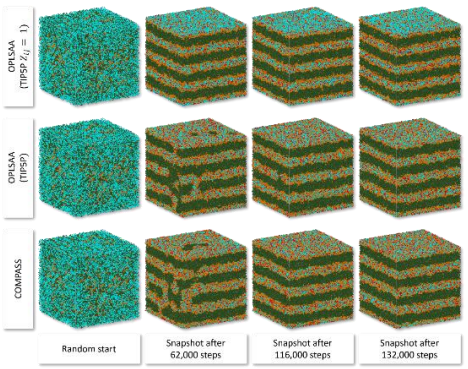
An automated pipeline for comprehensive calculation of intermolecular interaction energies based on molecular force-fields using the Tinker molecular modelling package is presented. Starting with non-optimized chemically intuitive monomer structures, the pipeline allows the approximation of global minimum energy monomers and dimers, configuration sampling for various monomer-monomer distances, estimation of coordination numbers by molecular dynamics simulations, and the evaluation of differential pair interaction energies.




The latter are used to derive Flory-Huggins parameters and isotropic particle-particle repulsions for Dissipative Particle Dynamics (DPD). The computational results for force fields MM3, MMFF94, OPLSAA and AMOEBA09 are analyzed with Density Functional Theory (DFT) calculations and DPD simulations for a mixture of the non-ionic polyoxyethylene alkyl ether surfactant $C_{10}E_4$ with water to demonstrate the usefulness of the approach.