A Calculation Pipeline for Differential Molecule Pair Interaction Energies

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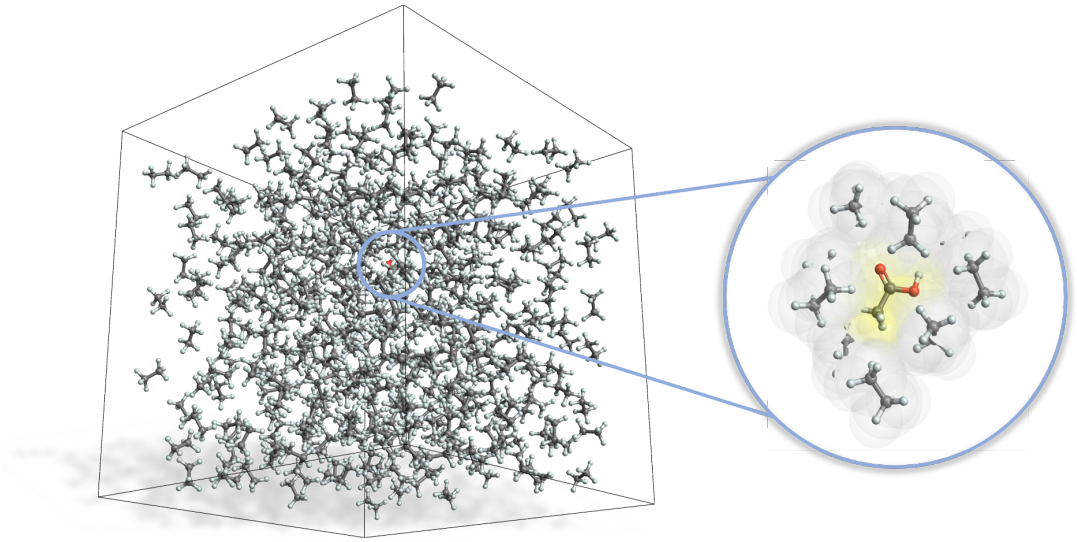
Dissipative Particle Dynamics (DPD) is a mesoscopic simulation technique for complex fluids and soft matter systems. Molecular Fragment DPD is a "bottom-up" variant, where particles are defined as small molecules with a molecular weight in the order of 100 Dalton. Larger molecules are composed of these "fragment molecule" particles, which are linked by harmonic springs to mimic covalent bonds and 3D spatial conformations. The conservative interaction between two DPD particles is characterized by an isotropic repulsion.



The open MIPET (Mesoscopic Interaction Parameter Estimation with Tinker) project aims at providing a force-field-based method for the consistent estimation of isotropic repulsions for pairs of small molecules which represent adequate DPD particles. A comprehensive set of these adequate particles is then utilized for biomolecular simulations containing peptides or proteins. Isotropic repulsions can be derived from Flory-Huggins interaction parameters which themselves are based on differential molecule pair interaction energies. The latter can be calculated from molecule pair coordination numbers and mutual molecule-molecule interactions [1]. These quantities are approximated by molecular mechanics simulations using the open TINKER package [2]. The full MIPET calculation pipeline is realized with the Wolfram Language [3] and uses the Mathematica system for execution and result evaluation.

[1] R. D. Groot, P. B. Warren, J. Chem. Phys., 1997, 107, 4423
[2] J. Rackers *et al.*, J. Chem. Theory Comput., 2018, 14, 5273
[3] Wolfram Mathematica: https://www.wolfram.com/mathematica/