A Calculation Pipeline for Differential Molecule Pair Interaction Energies

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Bottom-up variants of Dissipative Particle Dynamics (DPD), where particles can be defined as small molecules with a molecular weight in the order of 100 Daltons, allow the study of large (bio)molecular systems and supramolecular phenomena on the nanometre length and microsecond time scale. The conservative interaction between two DPD particles i and j is governed by an isotropic repulsion a_{ij} . Groot and Warren [1] have shown that a a_{ij} repulsion can be linearly related to the Flory-Huggins parameter χ_{ij} (see on the right), which itself can be derived from the coordination numbers Z_{ij} (i.e. the number of particles j surrounding particle i) and the inter-particle interaction energies E_{ij} . The MIPET (Mesoscopic Interaction Parameter Estimation using TINKER) project aims at establishing a force-field based calculation pipeline for fast approximation of coordination numbers and interaction energies using the Molecular Mechanics package TINKER [2].



Continuum Flory-Huggins Model







To calculate the differential pair interaction energy, the particles i and j are rotated in different orientations at various distances. The rotations are represented by the points on the spheres. In addition, at each position the second sphere is rotated around the imaginary axis between the particles. The global minimum non-bonded interaction energy is determined and used to Boltzmann average all the energy values found. Result is an optimal staggered configuration for the two methane molecules.



Visualisation of a step in a molecular dynamics simulation to estimate the coordination number Z_{ij} . The spatial environment of a single methane molecule (centre, yellow background), and thus the coordination number, is approximated by the number of the surrounding methane molecules (grey background) at the density of water.

0.6



Boltzmann averaged energy values for each set of the spatial arrangements described above plotted against the corresponding distance between particles i and j.



Coordination number Z_{ij} for methane surrounded by methane at the density of water, arithmetically averaged over the molecular dynamics simulation steps in femtoseconds.

Groot, R.D., Warren, P.B. Dissipative particle dynamics: Bridging the gap between atomistic and mesoscopic simulation. The Journal of Chemical Physics 107(11):4423-4435
Rackers, J.A., Wang, Z., Lu, C., Laury, M.L., Lagardère, L., Schnieders, M.J., Piquemal, J-P., Ren, P., Ponder, J.W. Tinker 8: Software Tools for Molecular Design. J. Chem. Theory Comput. 2018, 14, 10:5273–5289