Extension of molecular fragment based mesoscopic simulation to the biopolymer realm

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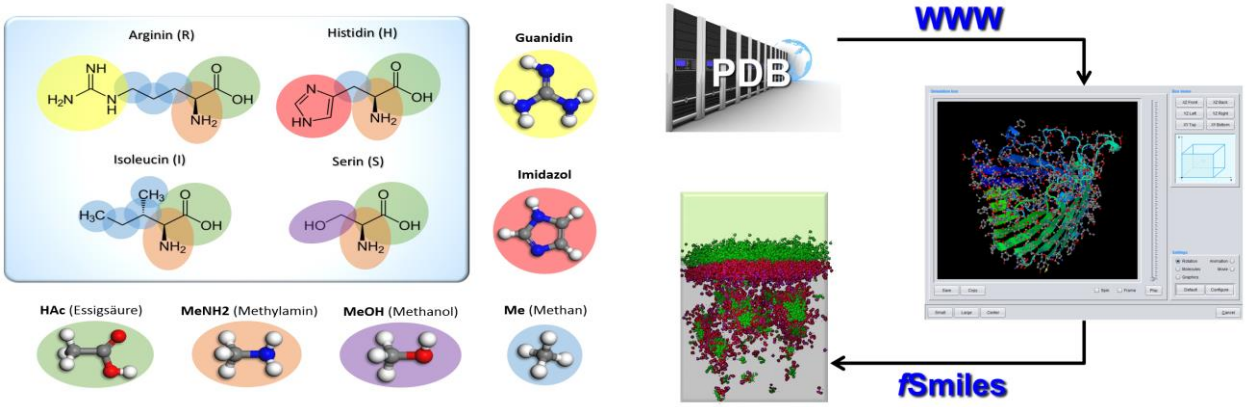
Dissipative Particle Dynamics (DPD) is an established simulation technique allowing the study of condensed matter on mesoscopic scales. Whereas its coarse-grained interacting units (beads) do not necessarily depend on distinct chemical compounds at all, the DPD variant Molecular Fragment Dynamics (MFD) makes use of specific molecules or molecular fragments. Recently MFD has been successfully applied for studying surfactant systems at the water-air interface [1]. This work aims at extending the MFD technique to the biopolymer realm of peptides and proteins.

To apply the MFD technique to biopolymers an adequate molecular fragment based description and an user interface for visualizing and editing the peptide or protein structure is required. The biopolymers are constructed from molecular fragments for all 20 proteinogenic amino acids including their charged species and disulfide bonds. The left figure shows the fragmentation scheme of selected amino acids. The editor allows the manual input of biopolymers from one-letter or three-letter amino acid codes. Additionally, for proteins the amino acid sequences and spatial data can be obtained from the Protein Data Bank (PDB) [2] (right figure). The visualization of structural data is based on Jmol [3]. All conversions are performed automatically including charges and spatial information.



MFD approximates the anisotropic molecular interactions in form of isotropic repulsion parameters. Since the structure of proteins is stabilized by anisotropic interactions like hydrogen bonds specific intramolecular potentials between fragments are defined to allow a flexible adjustment of the stiffness of the protein backbone.

[1] Truszkowski, A.; Epple, M.; Fiethen, A.; Zielesny, A.; Hubert, K. Molecular fragment dynamics study on the water-air interface behavior of non-ionic polyoxyethylene alkyl ether surfactants. *J. Colloid. Interface. Sci.* **2013**, 410, 140–145.

[2] Berman, H.M.; Westbrook, J.; Feng, Z.; Gilliland, G.; Bhat, T.N.; Weissig, H.; Shindyalov, I.N.; Bourne, P.E. The Protein Data Bank. *Nucleic Acids Res.* **2000**, 28, 235-242.

[3] Jmol: an open-source Java viewer for chemical structures in 3D. [online] http://www.jmol.org/ (accessed Jan 27, 2014).