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Structural changes in proteins at fluid-fluid interfaces

We study the behavior of several proteins at the air–water and oil–water interfaces by all-atom molecular dynamics. The proteins are found to change orientation and get distorted when pinned to the interface. This behavior is consistent with the empirical way of introducing the interfaces in a coarse-grained model through a hydropathy related force. Proteins couple to the oil-water interface stronger than to the air-water one. They diffuse slower at the oil-water interface but do not depin from it, whereas depinning events are observed at the other interface. The reduction of the disulfide bonds slows the diffusion down. We use the model to study interfacial protein layers and demonstrate existence of glassy effects as evidenced by slowing down of diffusion with increasing concentration of proteins. We also show that layers of two barley proteins, LTP1 and its ligand adduct LTP1b, flatten out at the interface and can make a continuous and dense film that should be responsible for formation and stability of foam in beer. The degree of the flattening depends on the protein - the layers of LTP1b should be denser than those of LTP1 – as well as on the presence of glycation and on the number of disulfide bonds.

Recent Publications

1. M Cieplak, D B Allen, R L Leheny and D H Reich (2014) Proteins at air-water interfaces: a coarse-grained approach. Langmuir 30(43):12888-96.
2. Y Zhao, M Chwastyk and M Cieplak (2017) Topological transformations in proteins: effects of heating and proximity of an interface. Scientific Reports 7:39851.
3. Y Zhao and M Cieplak (2017) Structural changes in barley protein LTP1 isoforms at air-water interfaces. Langmuir 33(19):4769-4780.
4. Y Zhao and M Cieplak (2017) Proteins at air-water and oil-water interfaces in an all-atom model. Physical Chemistry Chemical Physics 19:25197-25206.

Biography

Marek Cieplak is the Head of Laboratory of Biological Physics, Institute of Physics, Polish Academy of Sciences in Warsaw, Poland. He completed his MS from Department of Physics, University of Warsaw in 1973; PhD from Department of Physics, University of Pittsburgh in 1977; DSc from Department of Physics, University of Warsaw in 1984. He got his Professorial title in 1994. His fields of interest are condensed matter theory (spin waves, spin glasses, porous media, growth processes, atomic friction, river networks, nanofluidics, self-organized nanostructures) and biological physics (large conformational changes of biomolecules within coarse-grained models, especially as induced by stretching, proteins with knots and slipknots, protein folding, dynamics of virus capsids and other multi-proteinic structures such as a cellulosome, interaction of proteins with solids, proteins at air-water interface, modeling of proteasomes, inference of genetic networks from the microarray data).

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