COSMO*plex*: A new paradigm for simulating self-organizing systems

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The efficient combination of quantum chemical calculations with statistical thermodynamics COSMO-RS has become an important alternative to force-field based simulations for the accurate prediction of free energies of molecules in liquid systems [1]. While it originally was restricted to homogeneous liquids, it later has been extended to the prediction of the free energy of molecules in inhomogeneous systems as micelles, bio-membranes, or liquid interfaces, but these calculations were based on external input about the structure of the inhomogeneous system [2]. Recently an extension of COSMO-RS named COSMO*plex* has been developed, which allows for the self-consistent prediction of the structure and the free energies of molecules in self-organizing inhomogeneous systems. This extends the application range to many new areas, as the prediction of micellar structure and critical micelle concentrations, finite loading effects in micelles and bio-membranes, free energies and structure of liquid interfaces, micro-emulsions, and many more of similar problems, which often are of huge practical importance. COSMO*plex* [3] is approximately 10000 times faster than comparable molecular dynamics calculations and it is based on the same molecular interaction description as used in COSMO-RS. It does not require any re-parameterization, nor coarse graining. Thus it opens up completely new perspectives and possibilities for the simulation and screening of properties of inhomogeneous systems.

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