

Applications of the COSMO-RS and COSMOplex methods in formulation science

The COSMO-RS method is as highly efficient shortcut connecting quantum chemical information about the molecular polarity directly with macroscopic thermodynamic properties as solubility, partition coefficients, activity coefficients, or vapor pressures of a wide range of organic molecules in pure or mixed solvents. By that, COSMO-RS strongly increases the chemical “formulation space”, because new or even virtual molecules can be included in a screening for optimal formulations, for which the data would be missing otherwise. The COSMOquick tool even allows slightly less accurate, but very fast property predictions, avoiding the quantum chemical calculations, and thus it enables screening of almost unlimited virtual chemical spaces as solutes, solvents and additives.

In the recent years we succeeded to extend the COSMO-RS method to inhomogeneous liquids. This extension is named COSMOplex, because it enables the simulation of complex liquid systems as interfaces, surfaces, micelles and even micro-emulsions. A few applications of this exciting tool will be presented.