COSMO-RS: FROM QUANTUM CHEMISTRY TO FLUID PHASE THERMODYNAMICS AND MESOSCALE SYSTEMS

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The COnductor-like Screening MOdel (COSMO) \cite{1} and its re-implementations as CPCM \cite{2} are widely used as a most efficient and robust variant of the dielectric continuum solvation models in quantum chemical calculations. Considering that the novel and equivalent boundary conditions IEF and SS(V)PE \cite{3} are very closely related to COSMO, most likely the majority of quantum chemical calculations including solvation are nowadays performed with COSMO or COSMO derivatives.

By the success of COSMO, the computational chemistry community has missed to a large degree the Conductor-like Screeening MOdel for Realistic Solvation (COSMO-RS) \cite{5}. COSMO-RS combines the information gained by quantum-chemical COSMO calculations, i.e. mainly the surface polarization charge densities $\sigma$ resulting from such calculations, with an efficient and rigorous statistical thermodynamics treatment of interacting surfaces. By that COSMO-RS overcomes many of the severe limitations of the dielectric continuum solvation approach. It includes hydrogen bonding, entropy of solvation, and enables temperature dependence and mixture thermodynamics in a natural way. COSMO-RS treats solutes and solvents on the same footing, i.e. it requires no parameterization of solvents. Thus COSMO-RS improves the accuracy of continuum solvation models, and it extends the applicability of quantum chemically based calculations to many areas, which are not accessible at all using conventional solvation models. COSMO-RS has been taken up enthusiastically by the chemical engineering community for mixture thermodynamics calculations, and it has shown its great predictive potential by successful applications to areas as ionic liquids, pKa-prediction, drug-solubility, and even to meso-scale systems.

\cite{1} Klamt, A.; Schüürmann, G. J., Chem. Soc. Perkin Trans. 2 (1993) 799-805

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