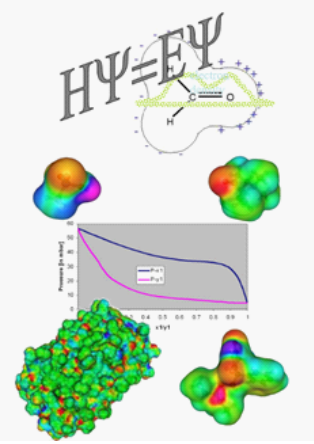
21st E. Hála Lecture

Ab initio Prediction to Phase Diagrams:
A Critical Review of the Alternative Pathways



While models for the accurate correlation methods for the description of fluid phase thermodynamic data and phase diagrams as UNIQUAC, NRTL, as well as equations of states have been developed in the chemical engineering thermodynamic community since many decades, the ab initio prediction of phase diagrams for compounds or mixtures, for which no experimental data is available, is a much less developed area of research. Within the chemical engineering approaches, essentially only the ASOG and UNIFAC methods are able to predict free energies of new mixtures, but by the group contribution approach they are based on the availability of good experimental data for similar compounds, and they are unable to handle intramolecular interactions of functional groups, as intramolecular hydrogen bonding, electronic push-pull effects, or steric shading. This prevents them from being applicable to multifunctional molecules as present in many areas of modern chemistry and pharmacy, and from the use for exploring really new areas of chemistry and compound classes. In this lecture the options for a more fundamental assessment of thermodynamic data in fluid phase thermodynamics, starting from electron distribution of molecules, *i.e.* from quantum chemistry, will be analyzed, and the special advantages and limitations of the COSMO-RS approach will be worked out.

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Dr. Klamt studied physics in Göttingen and received his first degree in 1984 in theoretical metal physics. Then he moved on to the Max-Planck-Institut for Metal Research in Stuttgart, where he received his PhD in 1987 with a thesis on 'States of small positively charged particles in metals'.

After his PhD he directly started to work at Bayer AG in Leverkusen in the area of Computational Chemistry. He specialized on solvation and physical property prediction and developed the methods COSMO and COSMO-RS, which meanwhile are widely used in the computational chemistry community. After being head of the central department for Computational Chemistry at Bayer for three years, he left Bayer in 1999 and founded COSMOlogic GmbH&Co.KG, Leverkusen, a company for Computational Chemistry and Fluid Phase Thermodynamics, Software and Consulting, which now has 16 co-workers. In December 2018 he handed over COSMOlogic to BIOVIA and now focusses on a number of ambitious research and development projects on COSMO-RS.

In 2005 he received his habilitation in Physical Chemistry at University of Regensburg, and in since 2012 he is honary professor, teaching courses for "Computational Fluid Phase Thermodynamics" every October in Regensburg.