

# Oral Contributions

## **[MS23-02] Co-crystal screening and other potential applications of COSMO-RS for crystallography**

A. Klamt

*COSMOlogic GmbH&CoKG, Leverkusen and Inst. of Phys. and Theoretical Chemistry, University of Regensburg.*

During the past decade the Conductorlike-Screening Model for Realistic Solvation (COSMO-RS) has been established as a reliable predictive tool for fluid phase thermodynamics. Although not being able to treat molecules in their solid crystalline form, COSMO-RS can nevertheless also be of great value for some aspects of crystal engineering. Different aspects will be discussed:

- Solvent screening and interaction analysis for finding interesting and diverse solvents for crystallization
- Estimate of  $\Delta G_{fus}$  based on COSMO-RS descriptors
- COSMOhkl for morphology engineering:  $\sigma$ -profiles of crystal faces and their free energy in solution
- Cocrystal Screening based on excess mixing enthalpy