

Keen thinker wanted

regarding the happiness of molecules in liquid systems

Very special permanent position available @ Dassault Systèmes (3DS) in former COSMOlogic

Summary: - Permanent position for an excellent theoretical scientist, preferably a theoretical physicist

- PhD or higher level of academic reputation expected
- Adequate industrial level salary
- Flexible work conditions
- Very exciting and challenging research topic

Detailed description: The COSMO-RS method is a combination of basic electrostatics and quantum chemical polarity information with an unusual model of statistical thermodynamics, predicting the free of almost any molecules in pure, mixed, and by a recent extension even in inhomogeneous, self-organizing liquids. It was invented by Andreas Klamt at Bayer and developed over 20 years in his company COSMOlogic. In many broad scale comparisons and several blind prediction challenges, COSMO-RS has proven to be about twice as accurate, and 10^4 -times faster than comparable molecular dynamics or Monte-Carlo simulations. Therefore, COSMO-RS is very popular in industry, while being a bit off the mainstream in academia.

For the completion of the development of a few really demanding projects (second-order COSMO-RS, COSMOplex, COSMO-RS for electrolytes) and for the conservation of the theoretical know-how, as well as for further extensions of the COSMO-RS theory, we are looking for a theoretical physicist, who has a really strong attitude to conceptual model building and for finding computationally efficient, affordable solutions. This requires that you are able to twist and tweak a complex theoretical problem for a while in your brain, before you start to write concrete code. The ability to code in FORTRAN is required. Furthermore, the candidate should know a bit about molecular interactions, without being a chemist.

After 20 years of independence, COSMOlogic has become part of Biovia, a world-leading company in computational chemistry software, and Biovia itself is part of 3DS (Dassault Systemes), one of the world's leading companies in simulation software, from airplanes down to molecules. Thus, the company offers – apart from attractive working conditions and salaries - an interesting and challenging environment, even beyond the small world of former COSMOlogic and BIOVIA. Andreas Klamt, the inventor and chief scientist in COSMO-RS theory, is going to retire in about two years. The here offered position has been specially created in order to train a successor as leading COSMO-RS scientist, working closely with Andreas during the initial two years.

If you are interested and sufficiently confident that you have the desired qualification, send an application by e-mail to

Prof. Dr. Andreas Klamt

Andreas.Klamt@3DS.com