UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

Theorie-Kolloquium WS 2023/24
Fr 20.10.2023, 14:00-15:30
MC 351 & online (URL in E-Mail)

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Molecular Theories meet Scientific Machine Learning - New Insights into Solvation Mechanisms

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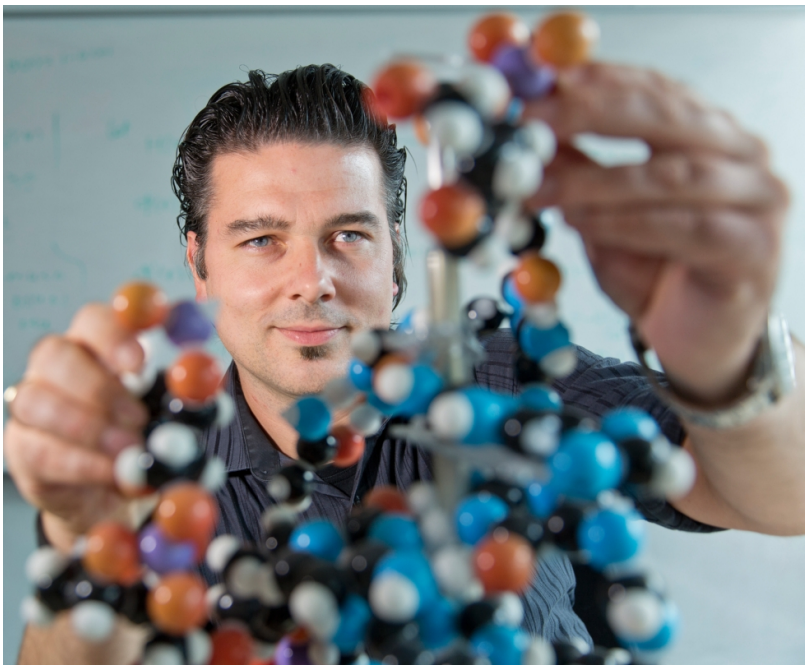

The molecular understanding of solubility mechanisms, solubilities and the interplay between the different components of a solution is of fundamental importance for basic research as well as for industrial applications. In particular, pharmaceutical processes and drug formulations depend on a variety of molecular mechanisms and principles. In recent years, considerable progress has been made in terms of fundamental understanding. Despite this progress, many issues remain unresolved, which is particularly detrimental for the optimization of development processes and for the quality and stability of drugs.

I will present recent molecular theories of electronic interactions in solutions. By combining this with explainable machine learning and statistical theories of solutions, the basic molecular mechanisms can be identified and the corresponding thermodynamic properties of the solutions can be understood and predicted. I will present these approaches for some examples such as for specific ion effects, stabilization and -destabilization mechanisms by co-solutes as well as other related empirical concepts. The advantages and limitations of these theories and approaches will be discussed in view of future developments.