universität innsbruck
Institut für Ionenphysik
und Angewandte Physik

Institutsseminar

Understanding Chemical Reactions: from Routine Calculations to Advanced Simulations

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Mechanistic studies, based on rapidly evolving and widely available density functional theory methods, are among the most standard applications of computational chemistry. Although these studies are performed routinely, accuracy is essential due to the well-known exponential dependence of the rate constants on the activation energies.

Based on real-life case studies from our research group I am going to demonstrate the relative importance of different free energy components starting from electronic energies up to the conformational entropy. I will also attempt to point out the inherent flaws of the routine approaches and show different strategies that are suggested to overcome these issues. Along these lines, I will show the advantages and limitations of on-the-fly ab initio and machine learning MD-based approaches via the available literature and first-hand experience.

HS F **17:15 Uhr** **01.02.2023**