Theoretical Chemistry
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Electronic Structure for Chemical Reactivity

In our research we develop and apply electronic-structure models and advanced simulation techniques to understand chemical reactivity from first principles.
We strive to bring these methods to a level of maturity, where *ab initio* and *in silico* design of highly efficient, selective and stable catalyst materials is possible.
Since we aim to understand, rationalize and extend experimental findings, we focus on the development of accurate models including relevant environmental conditions such as temperature effects and solvation.
Work in our group encompasses pen&paper theory, advanced scientific programming and the application of theoretical calculations and simulations using high-performance computing infrastructure.