Overview of Methane Activation and other Catalysis Research at the MSC

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The focus of the MSC catalysis group is the investigation, prediction and design of catalytic processes from first principles. The catalytic systems are normally of industrial interest, and range from homogeneous to heterogeneous to bio-organic (enzymatic) chemistry. Projects in the catalysis group are most often centered on mechanistic details, with the philosophy that a fundamental understanding of the underlying mechanism will enable the rational design of an improved system. In many cases the computational methodology necessary for a successful investigation has to first be developed in-house.

This talk will give an overview of the current research in the MSC catalysis group, with a particular emphasis on our theoretical exploration of catalysts for low-temperature activation and functionalization of C-H bonds. A short historical overview of this topic will be presented, followed by current approaches and recent results.

Computationally designed catalyst for the conversion of \( \text{CH}_4 + \text{H}_2\text{O}_2 \) to \( \text{CH}_3\text{OH} \) and \( \text{H}_2\text{O} \)