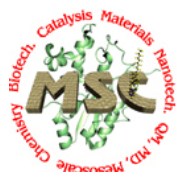
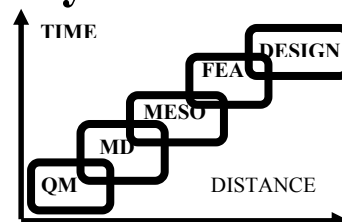


Mechanisms of and Improvements in Catalytic processes from First Principles Based Theory



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Advances in theoretical and computational chemistry are making it practical to consider using first principles based predictions to understand the mechanisms and improve catalytic performance for complex catalytic systems. We will illustrate this with recent applications to

- Mechanism Heterogeneous catalysis: oxidation and amoxidation on multimetal oxides
- Mechanism of dioxygen reduction reaction (ORR) on Pt alloy and non Pt cathodes
- Mechanism and design of new Organometallic reactions for converting methane to methanol

