

ABSTRACT:

Adventures of a Theoretician in the Land of Experimentalists or Computational Catalysis is Coming of Age

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The lecture will illustrate computational catalysis as a field of timely research which in recent years developed into a valuable tool for identifying reaction intermediates and unraveling mechanisms. As cornerstone for the successful solution of complex problems in catalysis, model building will be highlighted as joint responsibility of theoreticians and experimentalists alike. Chances and pitfalls will be discussed using case studies from heterogeneous and homogeneous catalysis. These examples will touch a variety of catalyst systems, mainly transition metal clusters and particles, but also metal-free molecular catalysis.