

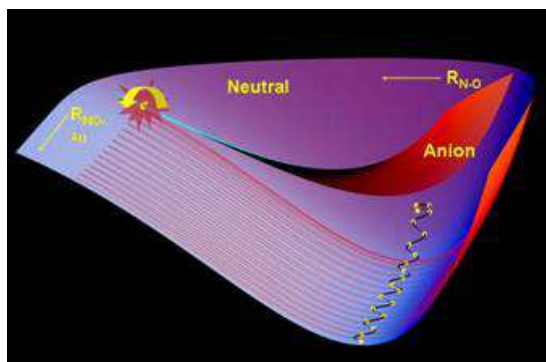
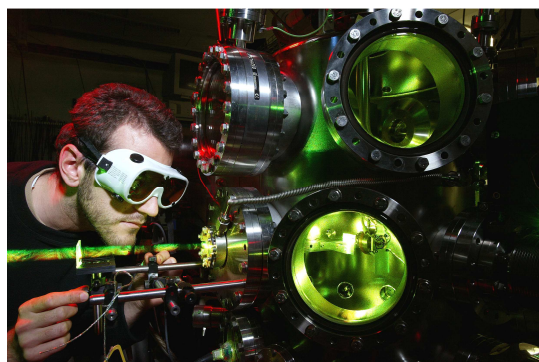
# State-to-State Dynamical Studies of Surface Chemistry and Energy Transfer



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While advances in computational chemistry have been profound, a predictive theoretical understanding of surface chemistry remains elusive even today. Our project targets two areas where more work is needed to help lay the ground work for the next generation of theoretical advances that: 1) go beyond the Born-Oppenheimer approximation and 2) adequately handle polyatomic reactivity. The experiments that are part of this project probe the dissociative chemisorption of HCl on Au(111) and state-to-state methane and acetylene scattering from transition metal surfaces to obtain detailed information about reactivity and energy transfer in gas/surface collisions.

Both the Wodtke group in Göttingen and the Beck group in Lausanne develop experiments to probe the dynamics of elementary chemical events at the gas/surface interface that can be compared to first principles theories. The Göttingen group specializes in state-to-state energy transfer studies via state-resolved detection of scattered species. The Lausanne group specializes in quantum state-resolved studies of chemisorption using detection of surface bound reaction products. By combining forces, our two groups will develop high quality benchmark data important to advancing our theoretical understanding of molecule-surface interactions.

## Representative publications:

Vibrationally promoted dissociation of water on Ni(111), P.M. Hundt, B. Jiang, M.E. van Reijnen, H. Guo, R.D. Beck, *Science* 344, 504, 2014, doi:10.1125/science.1251277

Quantum-State Resolved Gas/Surface Dynamics Experiments, in *Dynamics of Gas-Surface Interactions: Atomic-level Understanding of Scattering Processes at Surfaces*, R. D. Beck and A. L. Utz, Springer Series in Surface Science 50, 2013, doi:10.1007/978-3-642-32955-5\_8

*Controlling an electron transfer reaction at a metal surface by manipulating reactant motion and orientation*, Nils Bartels, Bastian C. Krüger, Christof Bartels, Daniel J. Auerbach, Alec M. Wodtke, Tim Schäfer, *Ang. Chemie – Int. Ed.* 2014, DOI: 10.1002/anie.201407051R1

*Observation of orientation dependent electron transfer in molecule-surface collisions*, Nils Bartels, Kai Golibrzuch, Christof Bartels, Chen Li, Daniel J. Auerbach, Alec M. Wodtke, Tim Schäfer, *Proceedings of the National Academy of Science* 110(44) 17738-17743 (2013) DOI 10.1073/pnas/1312200110.