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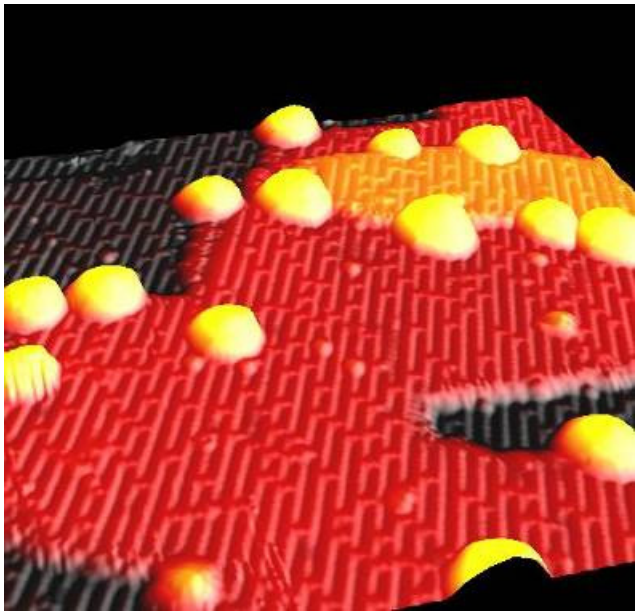
Research Interests: surface science, heterogeneous catalysis, scanning probe microscopy, mass spectrometry, model systems, metal-oxides, non-scalable size range.

Our research aims at providing a better fundamental understanding of the reactivity of metal-oxide surfaces. Our interest stems from a wish to explore the fundamental properties of the materials, as well as from a need for understanding their properties in sufficient detail to be able to improve their performance in technological applications. The mastering of adsorption/desorption and reactivity at the nanoscale is of utmost importance for society, being the cornerstone for technologies in various industries, environmental protection and sustainable energy production. We examine the influence of particle size and composition, and the metal-support interaction in heterogeneous catalysis within an atomistic approach. Selected reactions are studied, involving metal clusters supported on selected metal-oxide thin films or single crystalline supports.

STM image (3D rendered) of a well-defined single-crystalline rutile TiO2(110) surface on which gold atoms were evaporated at room-temperature. Nucleation and growth result in the formation of highly-dispersed nano-clusters. Such particles have been shown to catalyze CO oxidation very efficiently. The gold particles in this image are composed of a few tens of atoms with an average diameter of 2-3 nm.



SELECTED RECENT PUBLICATIONS

1. Oxygen Vacancies as Active Sites for Water Dissociation on Rutile TiO_2(110), R. Schaub, P. Thostrup, N. Lopez, E. Lægsgaard, I. Stensgaard, J.K. Nørskov, F. Besenbacher, *Physical Review Letters* **87** (26), 6104 (2001).
2. Oxygen-Mediated Diffusion of Oxygen Vacancies on the TiO_2(110) Surface, R. Schaub, E. Wahlström, A. Rønnau, E. Lægsgaard, I. Stensgaard, F. Besenbacher, *Science* **299**, 377 (2003).
3. Bonding of Gold Nanoclusters to Oxygen Vacancies on Rutile TiO_2(110), E. Wahlström, N. Lopez, R. Schaub, P. Thostrup, A. Rønnau, C. Africh, E. Lægsgaard, J.K. Nørskov, F. Besenbacher, *Physical Review Letters* **90**, 026101 (2003).
4. Electron Transfer-Induced Dynamics of Oxygen Molecules on the TiO_2(110) Surface, E. Wahlström, E.K. Vestergaard, R. Schaub, A. Rønnau, M. Vestergaard, E. Lægsgaard, I. Stensgaard, F. Besenbacher, *Science* **303**, 511 (2004).
5. Oxygen vacancies on TiO_2(110) and their interaction with H_2O and O_2: A combined high-resolution STM and DFT study, S. Wendt, R. Schaub, J. Matthiesen, E.K. Vestergaard, E. Wahlström, M.D. Rasmussen, P. Thostrup, L.M. Molina, E. Lægsgaard, I. Stensgaard, B. Hammer, F. Besenbacher, *Surface Science* **598**, 226 (2005).
6. Formation and Splitting of Paired Hydroxyl Groups on Reduced TiO_2(110), S. Wendt, J. Matthiesen, R. Schaub, E.K. Vestergaard, E. Lægsgaard, F. Besenbacher, B. Hammer, *Physical Review Letters* **96**, 066107 (2006).