Atomic-Scale Chemical Imaging via Combination of Scanning Tunneling and Electron Energy Loss Spectroscopies

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Purpose

- Direct spatial and temporal visualization of chemical reaction pathways to provide mechanistic understanding for catalytically important systems at atomic level
- Develop atomically resolved chemical imaging platform via combination of low-temperature scanning tunneling microscope (LT STM) with in situ molecular beam and ex situ electron spectroscopies

Expected Outcome

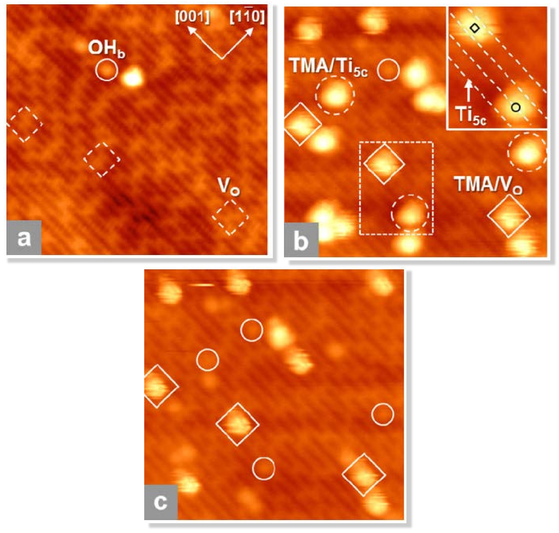
- Multimodal spectroscopic capability for chemically specific, surface-sensitive imaging at atomic/molecular level

Key Success

- Completed and successfully tested molecular beam device in situ coupled with LT STM for tip functionalization

Research Accomplishments

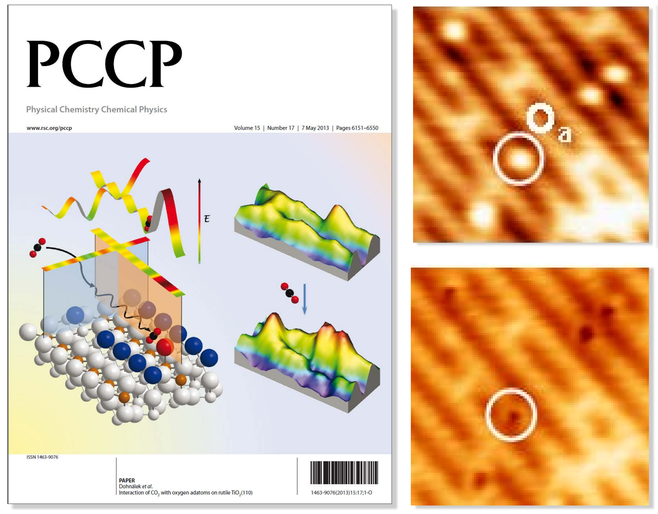
Suppressing Effect of Surface Point-Defects on Photoactivity



Wang Z et al. 2012. *Physical Review Letters* 109:266103.

- Chemical identity is inferred indirectly from known reagents and/or STM tip interactions
- Single-molecule tracking is critical for identifying active sites and visualizing reaction

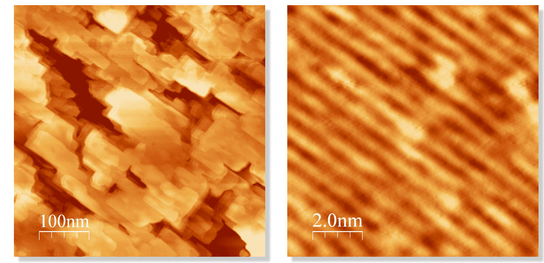
Adsorbate Identification via STM Tip Functionalization

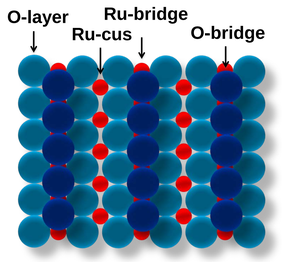


Lin X et al. 2013. *Physical Chemistry Chemical Physics* 15:6190.

- Functionalizing tips with well-defined terminations (CO, CO_2, OH, O_2) using molecular beam
- Exact knowledge of tip apex facilitates quantitative comparison with theoretical modeling
- Increased inelastic electron tunneling spectroscopy (IETS) resolution for specific, tip-imposed symmetries

Spectroscopic Studies of Adsorbates on Conductive Oxides





- RuO_2(110) selected as model oxide:
  - Metallic
  - Rutile (110) structure (as TiO_2(110))
- Reactor chamber built and tested
- Preparation conditions optimized
- First adsorption experiments are forthcoming

Next Steps

- Implement inelastic electron tunneling spectroscopy and benchmark against high-resolution electron energy loss spectroscopy
- Directly probe photocatalytic H_2O splitting on TiO_2(110) and CO_2 hydrogenation on RuO_2(110)

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