Engineering of surface polarons on rutile TiO_2(110), and CO adsorption on TiO_2(110)-supported Pd nanocrystals

Chi Ming YIM

Department of Chemistry and London Centre for Nanotechnology, University College London, United Kingdom

In this talk I will present some of our recent STM and DFT investigations of a number of interesting phenomena observed on the (110) surface of rutile TiO_2. In the first part of the talk, I will present our work on the behavior of oxygen vacancy (V_O) induced electron polarons at the rutile TiO_2(110) surface using low temperature STM imaging. We have found that the electrons are symmetrically distributed around V_O at 78 K; however, as the temperature is reduced, this distribution becomes increasingly asymmetric. Thus we directly visualize the temperature dependence of polaron hopping. By manipulating the lateral positions of individual V_O using tip voltage pulses, we were able to form a series of multimer V_O complexes, and showed that their associated excess electrons are also polaronic. Thus, we demonstrate that the configurations of polarons can be engineered, paving the way for the construction of conductive pathways germane to resistive switching devices.

In the second part of the talk, I will present our investigations on the adsorption of CO on TiO_2(110)-supported Pd nanocrystals, a model heterogeneous catalyst. The Pd nanocrystals prepared by physical vapour deposition in UHV, were ~20 nm wide, ~2 nm tall, and characterized by a (111) top facet. Dosing different amounts of CO onto the Pd/TiO_2 surface at 124 K lead to various CO overlayers forming on the nanocrystal (111) top facets. As well as overlayer structures previously imaged on the native Pd(111) surface, we observed two additional c(4×2)-2CO phases that are formed uniquely on the nanocrystals' (111) top facets. Our DFT calculations indicate that this is caused by the strain on the nanoparticle, induced by carpet growth across the substrate step-edges.