Special Materials Seminar

Thursday, May 12th at 12:15 pm, Room 1315

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Reactivity of anatase TiO_2(001) and rutile TiO_2(110) surfaces

It is conventionally suggested that the anatase TiO_2(001) surface is the most reactive one among the surfaces of the different polymorph of TiO_2, which have triggered tremendous studies on the synthesis of anatase (001)-surface-rich surface crystalline. However, the experimental results on this surface just give limited and indirect information so far. The anatase TiO_2(001) surface from mineral crystals, thin films, and chemically synthesized nanoparticles have been experimentally studied, but the reported results are quite contradicted. We believe that such a situation could be caused by the different samples used in these experiments. For instance, the existed impurity elements in a natural mineral anatase crystal could be an unavoidable factor, making its property different from the intrinsic one. To clearly understand the intrinsic activity of the (001) surface, a clean and well-controlled sample is needed. Epitaxially grown anatase TiO_2(001) thin films may provide contamination-free and well-controlled structure, which should be an appropriate sample to investigate the intrinsic activity of the surface.

Here, we have performed a systematic study on the characterization of the reactivity of epitaxially-grown anatase TiO_2(001)-(1´4) surfaces by means of microscopic and spectroscopic techniques in combination with first-principles calculations, in comparison with the results from the rutile TiO_2(110). We find that the defects of paired Ti atoms on the reduced surface are the active sites for H_2O, O_2, and methanol, but the perfect reconstructed lattice sites of the (001)-(1×4) surface are not very active. We suggest that the anatase TiO_2(001)-(1´4) surface is intrinsically quite inert because of the six-fold coordination of terminal Ti. By introducing two types of defects, that is, Ti pairs and O-bridged Ti pairs, through reduction or followed by re-oxidation treatments, the activity of the surface can be enhanced for thermal or photocatalytic dissociation of methanol.