ACTIVATION of CO_2 on OXIDE and METAL SURFACES

Richard Catlow

Dept of Chemistry, University College London, UK; School of Chemistry, Cardiff University, UK; Catalysis Hub, Research Complex at Harwell, Rutherford and Appleton Laboratory, Harwell, UK.

Understanding of activation mechanisms is crucially important in the development of catalytic processes for the conversion of CO_2 into chemical and fuels. We describe how computational methods based on Density Functional Theory (DFT) can be used to probe the structural and energetic aspects of these key processes for both oxide and metallic systems and for oxide supported metallic nano-clusters. We show how activated CO_2 may the be hydrogenated to form methanol and other products.