Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Internal Seminar

First Principles Studies of Electronic and Magnetic Properties of Surface Supported Atomic Clusters and Electrostatically Tunable Interaction of CO_2 with MgO Surfaces and Chemical Switching

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Adsorption of the $TaSi_{16}$ cluster on highly oriented pyrolytic graphite (HOPG) is studied using density functional methods. These calculations resolve some of the issues raised by the experiments of Shubita et al. (Chemical Characterisation of an Alkali-Like Superatom Consisting of a Ta-Encapsulating Si_{16} Cage. *J. Am. Chem. Soc. 2015, 137, 14015−14018*) and provide additional insights into the system.

In another study, Electric field-assisted CO_2 capture using solid adsorbents based on basic oxides can immensely reduce the required energy consumption compared to the conventional processes of temperature or pressure swing adsorption. In this work, we present first-principles density functional theoretical calculations to investigate the effects of an applied external electric field (AEEF) within the range from −1 to 1 V/ Å on the CO_2 adsorption behaviour on various high and low-index facets of MgO. When CO_2 is strongly adsorbed on MgO surfaces to form carbonate species, the coupling of electric fields with the resulting intrinsic dipole moment induces a 'switch' from a strongly chemisorbed state to a weakly chemisorbed or physisorbed state at a critical value of AEEF.

Wednesday, Apr 16th 2025

14:45 Hrs

Seminar Hall, TIFRH