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

Students' Annual Seminar

Modelling the interaction of CO_2 on Gold beyond classical force field simulations

Nandana Pal Chowdhury

Previous force field based simulations were found to be inadequate to model the adsorption of pure CO_2 fluid on Au {111} surface. In the first part of the talk, I will discuss the preliminary results on the deviations observed upon modelling the system with ab initio molecular dynamics (AIMD), especially the extent of surface distortion and electron density polarisation effects that are missing from the force field simulations. In the second project, our goal is to model the chemisorption of CO_2 on charged single crystalline Au surfaces ({111}, {110}), which has been shown to be the rate determining step for the conversion of CO_2 to CO. Additionally, it has been suggested that grain boundaries are able to catalyse this process selectively over proton reduction. However, one could generate a large variety of grain boundaries between two misaligned grains. In the last part of my talk, I will discuss how to generate the grain boundaries and provide a quantitative measure by which one can identify how different they are.

Monday, May 6th 2024

17:00 Hrs (Tea / Coffee 16:45 Hrs)

Seminar Hall, TIFR-H