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

Seminar

Adsorption of Carbon Dioxide on Planar Gold Surface

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Experimental studies show that the adsorption of CO_2 on Au(111) surface follows a type II/III isotherm irrespective of surface roughness. Previous computational studies based on classical molecular dynamics with non-polarizable force field parameters shows a type I behaviour and hence, fail to capture the nature of the adsorption isotherm. This discrepancy between experiment and theory has been ascribed to surface irregularities. In this study we perform classical molecular dynamics with non-polarizable and polarizable force fields for CO_2 and Au while computing the Au/CO_2 interactions employing traditional mixing rules. All these different simulations mirror the above failure and show type-I behaviour for CO_2 adsorption. Going back to the basics, we discovered that potential energy curves for the adsorption of a single CO_2 molecule on Au(111) surface obtained with classical force field parameters differ significantly from the corresponding curves generated with density functional theory (DFT) indicating that the solid-fluid interaction, modelled by mixing rules, is probably incorrect. We have generated explicit Au/C and Au/O Lennard-Jones parameters by benchmarking against Van der Waals corrected DFT. The change in adsorption capacity with the bulk density obtained from the MD simulations with these new parameters shows clear multilayering at lower densities of CO_2.

Tuesday, Jan 23rd 2024

11:30 Hrs (Tea / Coffee 11:15 Hrs)

Auditorium, TIFR-H