School of Nano Science

School of PHYSICS

IPM Condensed Matter & Statistical Physics Group

Weekly Seminar

Computational Studies of the Adsorption of Hydrazine on Cu Surfaces: A Dispersion-Corrected DFT Study

Invited Speaker:

Dr. Saeedeh S.Tafreshi

University College London (UCL)

Abstract:

The copper-hydrazine interface is of importance in a number of applications, and in order to produce copper nanoparticles with specific properties or improve copper electrodes for more efficient fuel cells like proton exchange membranes fuel cells (PEMFC), or investigate the catalytic activity of Cu towards hydrazine (N_2H_4) decomposition for the production of hydrogen, nitrogen and ammonia, we need to gain fundamental understanding of the interactions between N_2H_4 and Cu surfaces. The computational study of the molecular adsorption of hydrazine on low-index perfect and defective copper surfaces has been investigated, using the density functional theory calculations with long-range dispersion correction (DFT-D2) resulting in significant enhancement of molecule-substrate binding. Furthermore, we have simulated the dissociative adsorption of hydrazine on the planar and stepped Cu(111) surfaces. We found that hydrazine prefers to form NH_2 via N–N bond decoupling, where the NH_2 molecule reacts fairly easily with co-adsorbed NH_2 to form NH_3, as well as with N_2H_X (x=1–4) by subtracting hydrogen to produce NH_3 and N_2 molecules. We have constructed a microkinetic model to develop our understanding of the catalytic process of N_2H_4 dissociation on the planar Cu(111) surfaces. The temperature programmed reaction and batch reactor simulations were simulated, showing that the NH_3 and N_2 are the dominant gaseous products, while H_2 is the minor gaseous product.

Wednesday, 14 Tir 1396 (July. 5, 2017), 14:00-15:00

Seminar Room (classroom A), Farmanieh Building, IPM