Weekly Seminar

Importance of Long-Wavelength Phonons for Dissociative Chemisorption: N2 on Ru(0001)

Invited speaker:

Dr. Hossein Tahmasbi

Department of Physics, Institute for Advanced Studies in Basic Sciences (IASBS)

Abstract:

Ab initio molecular dynamics (AIMD) simulations can describe reactions of molecules with metal surfaces accurately. However, the computational costs of AIMD have limited its applications to the systems with reaction probabilities higher than 1%.

Recently, Neural network potentials (NNPs) have allowed overcoming this limitation but small cell sizes (typically 3×3) inherited which resulting in a rather coarse description of the phonon continuum by phonons of only very few different wave vectors (typically 9). In this work, based on NNPs, we increase systematically the set of phonon wave vectors using larger cells in simulations. Therefore, the role of long-wavelength phonons in the reaction probability and thus energy dissipation at low incidence energies is investigated. The results show that the long-wavelength phonons increase the reaction probability at low incidence energies and constitute the largest contribution to the energy uptake of the surface.

Wednesday, 6 Shahrivar 1398 (August 28, 2019), 14:00-15:00

Seminar Room (Classroom A), Farmanieh Building, IPM