Stony Brook University
The Graduate School

Doctoral Defense Announcement

Abstract

Theoretical Approach of Water/Surfaces Interactions

By

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Much effort is being devoted to the understanding of water-substrate interactions at metallic or semiconducting surfaces with catalytic properties.
Confined water represents a great interest for physicists and chemists interested in state-of-the-art technologies such as, fuel cells where the rates of proton have to be controlled, nano-sensors, heterogeneous catalysis, or nano-fluids.
Creation of hydrogen gas from water dissociation, also remains an important challenge in order to complete the cycle of CO2 free green energies production. Photocatalytic processes, with semiconducting substrates such as GaN 10$\underline{1}$0 seem to represent strong candidates towards this achievement.
This work focuses on the investigation of water-substrate interactions. It is mainly directed from first-principle calculations with molecular dynamics simulations. The nature of the hydrogen bond is broadly discussed and comparisons between water-water and water-substrate are proposed.
Interesting features of spontaneous metal polarization are also put in evidence and electrochemical mechanisms are explained.

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Place: B 131