

**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 CO<sub>2</sub> free green energies production. Photocatalytic processes, with semiconducting substrates such as GaN 1010 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.

**Date:** December 14, 2011

**Time:** 2:00 pm

**Place:** B 131

**Program:** Physics

**Dissertation Advisor:** Maria Victoria Fernandez- Serra