University of Notre Dame
College of Science
Department of Physics

CONDENSED MATTER SEMINAR

Simulating the liquid-solid interface: first steps with SCC-DFTB

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Theoretical modeling and understanding of the reaction mechanisms involved in catalysis at gas-solid interfaces has advanced significantly with the use of various flavours of DFT. However, processes like photocatalysis that take place at lower temperatures require ways of describing reactions across the liquid-solid interface, under the influence of the dynamics of the liquid. Furthermore, this need for large systems is countered by a requirement for quantum chemical accuracy.

I will present some first steps in the direction of modeling the water / titanium dioxide interface with the Self-Consistent Charge Density Functional Tight Binding method. Although this method has been around for some time, parameters for describing the interactions in systems including materials such at TiO_2 have only recently become available and present an opportunity for investigating the liquid-solid interface in sufficient depth.

ALL INTERESTED PERSONS ARE CORDIALLY INVITED TO ATTEND