



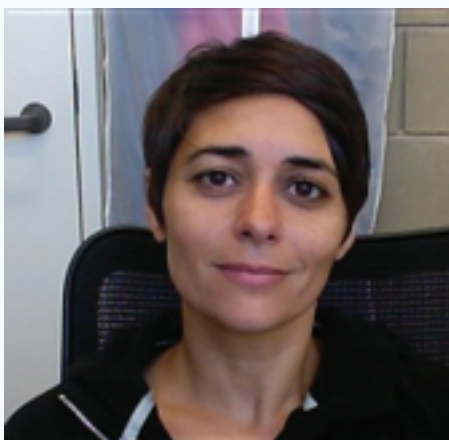
HARVARD

John A. Paulson
School of Engineering
and Applied Sciences

APPLIED PHYSICS COLLOQUIUM

4:00 P.M., Friday February 24th in Pierce 209

Understanding water/solid functional interfaces for photocatalysis and electrochemical applications



Marivi Fernandez-Serra
Stony Brook University
Physics Department

In this talk I will review our current efforts on understanding the physics of liquid water and the interaction of water with functional semiconductor and metallic surfaces using ab initio molecular dynamics methods. I will present the state of the art of current simulations and the challenges we face, focusing on two specific problems: the description of aqueous solvated electrode surfaces and the simulation of polar surfaces in aqueous environments. In particular I will show how the physics of ferroelectric and dielectric superlattices is strongly related to the physics that describes the behavior of water at polar interfaces.

Host: Alan Aspuru-Guzik