

MAR17-2016-020521

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Using density functional theory to solve complex problems: from liquid water to dark matter

MARIVI FERNANDEZ SERRA, State Univ of NY- Stony Brook

In this talk I will review our current efforts on understanding the physics of liquid water and the interaction of water with functional semiconductor 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 electron-electron interactions using semilocal density functionals and the role of nuclear quantum effects. I will finish the talk introducing our work in the field of dark matter detection, showing how electronic structure theory is a tool that can easily be used by high energy theorists to evaluate their predictions about the interactions of dark matter particles with electrons in solids, opening a bridge between two otherwise very distant communities.