

Abstract for an Invited Paper
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Predictive simulations of semiconductor nanostructures

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Ab-initio simulations are playing an increasingly important role in understanding matter at the nanoscale and in predicting with controllable, quantitative accuracy the novel and complex properties of nanomaterials. A microscopic, fundamental understanding of nanoscale phenomena is very much in demand, as experimental investigations are sometimes controversial and usually they cannot be explained on the basis of simple models. In this talk, *ab-initio* molecular dynamics simulations and quantum monte carlo calculations of semiconductor nanoparticles will be presented, with focus on electronic and optical properties and on the microscopic structure of surfaces at the nanoscale. The characterization of nanoscale surfaces and interfaces is of paramount importance to predict the function of nanomaterials, and eventually their assembly into macroscopic solids, and it is still very challenging from an experimental standpoint, due to the lack of appropriate imaging techniques. The presentation will focus on Si, Ge, SiC nanoparticles and nanodiamond, and in addition we will discuss several results for II-VI dots and rods. (*) Work done in collaboration with G.Cicero, E.Draeger, J.Grossman, F.Gygi, D.Prendergast, A.Puzder, J.-Y.Raty, F.Reboredo, E.Schwegler, A.Williamson This work was performed under the auspices of the US Department of Energy by the University of California at the LLNL under contract no W-7405-Eng-48