

Abstract Submitted
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QMC calculations of the optical gaps of Ge Nanoclusters using CPPs JORDAN VINCENT, Physics Dept. at UIUC, JEONGNIM KIM, NCSA/MCC at UIUC, RICHARD MARTIN, Physics Dept. at UIUC — Quantum Monte Carlo (QMC) calculations of the optical gaps of hydrogen-passivated Ge clusters of size 1-3 nm are presented. Although QMC methods are the most accurate methods known for interacting electrons, there are outstanding challenges in applications to materials containing heavy atoms such as Ge. The replacement of core-electrons by a pseudopotential (PP) is a primary limiting factor for the accuracy of current methods. Previous work has proposed that atoms like Ge with shallow core states can be treated using a Hartree-Fock PP plus a core-polarization potential (CPP) to account for core-valance correlation at a many-body level[1]. The goal of our work is to quantify the effect of the CPP and to predict the properties of Ge clusters in comparison to previous results[2] calculated using the time-dependent local-density approximation (TDLDA) on the same structures. [1] A. Nicklass and H. Stoll, Mol. Phys. 86, 317 (1995). [2] A. Tsolakidis and R.M. Martin, TBP. Supported by NSF DMR-03 25939 ITR.

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