Quantum Monte Carlo Calculations of Excitations in Hydrogenated Germanium Clusters JORDAN VINCENT, Physics Dept. at UIUC, JEONGNIM KIM, NCSA/MCC at UIUC, RICHARD MARTIN, Physics Dept. at UIUC — Quantum Monte Carlo (QMC) calculations are presented for energies of ground and excited states of Ge atom and hydrogen passivated closed-shell molecules and clusters: GeH4, Ge2H6, Ge5H12, Ge10H16 and Ge29H36. We compare the results for excitations with previous QMC and time-dependant Density Functional Theory (TD- DFT) done for the corresponding Silicon clusters [1,2]; in particular; we find that preliminary results for lowest excitation enregy of Ge29H36 5.08[29]eV is lower than the gap 5.4eV reported for Si[2]. Core-valence partitioning for Ge is implemented by replacing the core-states with a Hartree-Fock pseudopotential plus a Core Polarization Potential (CPP)[3]. Core-valence correlation treated by the CPP is shown to be essential for accurate atomic energies and significant for the molecules, but smaller in the clusters. [1] Porter et. al., PRB 64, 035320 (2001). [2] Williamson et. al., PRL 89, 196803 (2002). [3] Shirley and Martin, PRB 47, 15413 (1993)

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