Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

***Ab Initio* Studies of Si_mGe_n(m+n $\leq$ 5) Nanoclusters**[1] SARAH DUESMAN, ASOK RAY, University of Texas at Arlington — Electronic and geometric structure properties of Si_mGe_n(m+n ≤ 5) nanoclusters have been investigated using hybrid density functional B3LYP, 6-311G (3df, 3pd) basis set, and the GAUSSIAN 03 software. For the Si atom, the computed values of the ionization potential and electron affinity are 8.11 and 1.10eV, and for the Ge atom, the values are 7.90 and 1.14eV. The experimental values are 8.15, 1.39, 7.90, and 1.23eV, respectively. Various possible geometries have been spin-optimized to determine the global minimum for each nanocluster. We will present the electronic and geometric structures of the isomers of each nanocluster, including bond length, symmetry group, electronic state, binding energy, HOMO-LUMO gap, ionization potential, and electron affinity. In addition, the harmonic frequencies, fragmentation energies, average coordination number and Mulliken atomic charges will also be discussed for the ground states of the nanoclusters.

[1]This work is partially supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525).

Sarah Duesman
University of Texas at Arlington

Date submitted: 23 Nov 2010 Electronic form version 1.4