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Structural Analysis of Bonding in Au-Ge Clusters DANIELLE MCDERMOTT, KATHIE NEWMAN, University of Notre Dame — The study of Gold-Germanium clusters is important in understanding systems such as gold catalyzed nanowire growth. Of particular concern is the bonding behavior between the two chemical elements, one tending to form metallic bonds, the other covalent. DFT calculations and Conjugate Gradient relaxations were performed on clusters ranging in size from 50 to 150 atoms using the SIESTA code to find the geometries of metastable states. Emphasis has been placed on developing accurate and dependable bases to be used to study nano-sized systems. The binding energy, coordination number, bond lengths and bond angles are studied as a function of the size and composition of Ge-Au clusters. We will discuss a nanoscale "phase diagram" for gold and germanium and will also discuss the topology of the bonding network.

Kathie Newman
University of Notre Dame

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