Assembling Ge$_6$Au$_N$ Structures From Ge$_6$ Building Blocks

KATHIE NEWMAN, DANIELLE MCDERMOTT, University of Notre Dame — Unusual crystalline germanium materials useful for optical and semiconducting devices can be synthesized through precursors of small anionic Ge clusters. Furthermore, a successful catalyst of germanium nanowires are gold nanoparticles, yet theoretical methods to describe the Au-Ge interaction are incomplete. Thus we apply Density Functional theory to a series of neutral and anionic Ge$_6$ clusters linked with gold atoms to form Ge$_{12}$Au$_N$ molecules where $N = 0,1,2,3$. We present the lowest energy Conjugant Gradient relaxed clusters and perform short Molecular Dynamics simulations to evaluate their stability. The gold-germanium bondlengths and angles affect the electronic properties of the molecules, which we characterize with total and partial Density of States and the COHP (Crystalline Orbital Hamiltonian Population) method. The electronic structure reveals a stability motif in which gold donates stabilizing electrons. This suggests how Ge$_6$ can form extended structures of Ge$_6$Au$_N$ such as 1D chains and 2D surfaces.

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