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Assembling Ge_6Au_N Structures From Ge_6 Building Blocks[1]
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Unusual crystalline germanium materials useful for optical and semiconducting devices can been 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_6Au_N such as 1D chains and 2D surfaces.

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