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Ab initio **study of dimer and one-dimensional chain structures of M@Au$_{12}$ (M = W, Mo) clusters** SORA PARK, GUNN KIM, YOUNG-KYUN KWON, Kyung Hee University — Using density functional theory, we investigate the structural and electronic properties of the dimer and one-dimensional (1D) chain structures composed of metal-encapsulated Au_{12} nanoclusters (M@Au_{12}, M = W, Mo) with icosahedral (I_h) and cuboctahedral (O_h) symmetries. We consider various dimer configurations with different compounds and symmetries to find the most stable dimer structure in each case. We find that during dimerization (either homogeneous or heterogeneous dimer), Au atoms in the one cluster tend to form triangular bonds with counterpart Au atoms in the other. By maximizing the number of Au-Au bonds by dimerization, any cluster is stabilized by about 3 eV. We further find their stable 1D chain structures by considering various 1D chain configurations with different compounds and symmetries. Our results demonstrate that the spin-orbit coupling effects are significant on the electronic and magnetic properties as well as the structural stability due to $5d$ electrons in a transition metal atom M of the M@Au_{12} nanocluster. We also present interesting differences in electronic and magnetic properties between I_h- and O_h-symmetric 1D polymerized M@Au_{12} chain structures.

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