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Ab initio DFT studies on dimerization and one-dimensional (1-D) polymerization of $M@Au_{12}$ (M = W, Mo) clusters

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Using ab initio density functional theory, we investigate the dimerization and one-dimensional (1-D) polymerization of metal-encapsulated gold nanoclusters, $M@Au_{12}$ (M=W, Mo) and their structural and electronic properties. $M@Au_{12}$ clusters with a magic number 13 can form icosahedral and cuboctahedral structures. We consider various dimer configurations with different compounds and symmetries to find the most stable dimer structure in each case. Au atoms in the one cluster, which participate directly in dimerization, tend to form triangular bonds together with counterpart Au atoms in the other. It is found that both $M@Au_{12}$ and $M@Au_{12}$ clusters are stabilized by about 3 eV due to dimerization. We also calculate and compare the electronic and magnetic properties of different dimerized clusters. Based on our investigation on dimerization, we further study on 1-D polymerization of $M@Au_{12}$ with different compounds and symmetries. We will also discuss their formation energies as well as their electronic and magnetic properties.