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Quantum-Mechanical Study of Small Au_2Pd_n (n=1～4) Clusters

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Abstract: Gold-doped palladium clusters, Au_2Pd_n (n=1～4), are investigated using the density functional method B3LYP with relativistic effective core potentials (RECP) and LANL2DZ basis set. The possible geometrical configurations with their electronic states are determined, and the stability trend is investigated. Several low-lying isomers are determined, and many of them are in electronic configurations with a high-spin multiplicity. Our results indicate that the palladium-gold interaction is strong enough to modify the known pattern of bare palladium clusters, and the lower stability as the structures grow in size. The present calculations are useful to understanding the enhanced catalytic activity and selectivity gained by using gold-doped palladium catalyst.

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Key words: Au-Pd clusters, geometrical configuration, density functional method

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