

Abstract Submitted  
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**The peculiar distribution pattern of Pd on the PdAu bimetallic nanoclusters**<sup>1</sup> DINGWANG YUAN, University of California, Irvine, XINGAO GONG, Fudan University, RUQIAN WU, University of California, Irvine — Through systematic density functional calculations, we found that Pd atoms in PdAu nanoclusters may only take the (111) facets while leave the (001) facets with pure Au. This is promoted by the tendency that Pd prefers to form bonds with Au, rather than Pd. The segregation from the (001) facet to the (111) facet appears to occur easily. The local activity of Pd somewhat depends on the size of cluster and site of substitution. The peculiar distribution pattern of the active constituent should strongly alter the chemical properties of bimetallic nanoclusters toward catalyzing reactions.

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