Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Interaction of Magic Gold Cluster with Si60 Cage YOSHI KAWAZOE, Tohoku University, QIANG SUN, QIAN WANG, PURU JENA, Virginia Commonwealth University — Both Au clusters and Si clusters individually are important subjects in chemistry, physics, and materials science. It is very interesting to study the interactions between these two technologically important systems. In this paper, first-principles studies are performed on $Au_{12}W@Si_{60}$ by using projector-augmented wave (PAW) method and generalized gradient approximation for the exchange-correlation energy. The geometry, electronic structure, orbital hybridization, and charge transfer are discussed. It has been found that the magic $Au_{12}W$ cluster actively interacts with Si, and Si_{60} cage structure can be stabilized. Meanwhile the metal cluster is dissociated when encapsulated in Si60 cage, and charge is transferred from Si cage to the metal atoms. The present study suggests that due to the special properties of Au itself, the magic gold clusters have both energetic stability and chemical activity and can be used to design novel nano structures and nano devices.

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Date submitted: 22 Nov 2004 Electronic form version 1.4