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Rare Earth Doped Magnetic Clusters of Gold for Medical Application BRAHM DEO YADAV, VIJAY KUMAR, Dr. Vijay Kumar Foundation — In recent years gold clusters have been studied extensively due to their unusual properties and applications in cancer treatment and catalysis. Small gold clusters having up to 15 atoms are planar as shown in figure 1. Thereafter a transition occurs to 3D structures but the atomic structures continue to have high dispersion. Doping of these clusters could transform them in to new structures and affect the properties. Gold clusters with cage structures such as $W@Au_{12}$ can be prepared with large highest occupied-lowest unoccupied molecular orbital (HOMO-LUMO) gap by doping with a transition metal atom such as W. By changing the transition metal atom, cage structures of different sizes as well as different HOMO-LUMO gaps can be formed which could be useful in different optical applications. In these structures gold clusters are generally non-magnetic. However, it is also possible to form magnetic clusters of gold such as Gold clusters have been found to be good for cancer treatment. We have performed ab initio calculations on doping of rare earths in small gold clusters to obtain magnetic clusters using projector augmented wave pseudopotential method within generalized gradient approximation for the exchange-correlation energy. Elemental gold clusters having up to 15 atoms are planar and thereafter 3D structures become favorable. We have explored the changes in the growth behavior when a rare earth atom is doped and studied the variation in the magnetic behavior as a function of size. Our results suggest that gold clusters may have twin advantage of treating cancer as well as be helpful in magnetic imaging such as by MRI.

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