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# Structure and Electronic Properties of Aunpt (N = 1–8) Nanoalloy Clusters: The Density Functional Theory Study

P. Ranjana, **Tanmoy Chakrabortyb,c**

a. Department of Mechatronics Engineering, Manipal University Jaipur, Dehmi Kalan, Jaipur, 303007, India

b. Department of Chemistry, School of Engineering, Presidency University, Bengaluru, 560064, India

c. Department of Chemistry, Manipal University Jaipur, Dehmi Kalan, Jaipur, 303007, India

**Abstract**

The study of bimetallic nanoalloy clusters is of considerable interest due to its interesting electronic, optical, magnetic and catalytic properties. The geometrical structure and electronic properties of AunPt (n = 1–8) nanoalloy clusters are studied by using the density functional theory methodology. The result exhibits that the ground-state configurations of AunPt clusters favour planar confirmation in this molecular range. The most stable cluster is Au3Pt, which is having rhombus structure with symmetry group C2v and can be considered as building blocks for developing large clusters. The computed HOMO-LUMO energy gap of Au3Pt nanoalloy cluster is 1.741 eV. The energy gap in this particular range supports the use of bimetallic clusters as nonlinear optical devices and optoelectronic materials. The DFT-based global descriptors viz. HOMO-LUMO energy gap, electronegativity, hardness, softness and electrophilicity index are also studied. The computed HOMO-LUMO energy gap and chemical hardness exhibit a pronounced odd-even oscillation behaviour as a function of cluster size, n.

**Keywords:**

Density functional theory Bimetallic clusters AuPt, Structure HOMO-LUMO energy gap, Hardness Odd-even oscillation, Modeling and simulation

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