

## **A theoretical study on interaction of proline with gold cluster**

Authors: SANDHYA RAI, N V SURESH KUMAR and HARJINDER SINGH

Journal: Bulletin of Materials Science, (2011), in press.

### **Abstract:**

**Interaction of proline with gold cluster was studied using density functional theory (DFT). Two types of mixed basis sets UB3LYP/6-311++G  $\cup$  LANL2MB and UB3LYP/6-311++G  $\cup$  LANL2DZ were used for optimization of complex structures. Proline interacts with gold cluster either through one anchor bond, N-Au or an anchor bond O-Au associated with a non-conventional O-H...Au hydrogen bond. Among these interactions, higher tendency for interaction is seen with Au cluster through amide terminal. Natural bond orbital analysis (NBO) is used to substantiate the results.**