# Core-level shifts in gold nanoclusters

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The evolution of the core-states from an individual atom to bulk through cluster has been investigated. The core-level shifts (CLS) have been analyzed in nanoclusters and their origin has been explained. We have analyzed how CLS depend on the morphology of the nanocluster. In Fig.1 CLS for icosahedral nanoclusters are provided. Undercoordinated surface atoms demonstrate negative shifts and compressed internal atoms have positive shifts. We have shown that for all morphologies the dependence of the CLS on the cluster size is a non-monotonic function and it approaches the binding energy of the bulk system with increase of the cluster size. Which means that different morphology exhibit maximum of CLS at different sizes. The origin of the CLS has been explained by the behavior of the d-band. Our calculations have shown that positive CLS in nanoclusters observed in many experiments can be due to both: confinement effect and internal stress. Moreover, we have shown that small clusters have the largest CLS. The main contribution of the CLS were distinguished: lattice parameter, coordination and confinement effect. The contributions were explained by the change of the d-band. From our calculations we predict that in XPS spectra icosahedral and octahedral clusters should have more narrow positive peak.

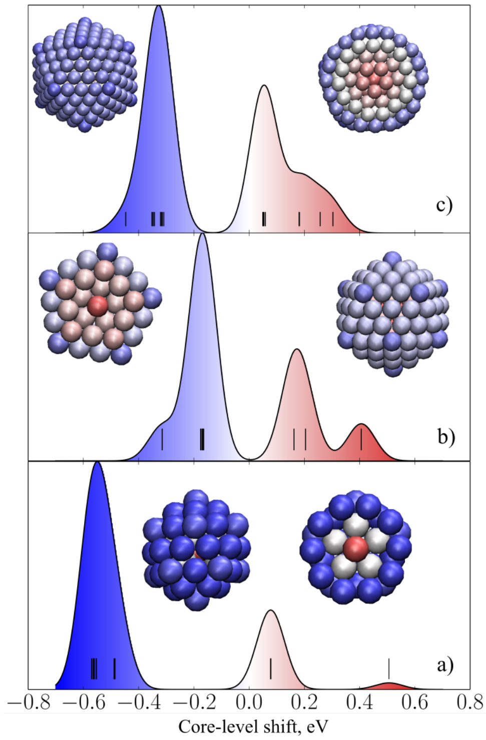


Figure 1: CLS in icosahedral nanoclusters: 55, 147 and 309 atoms. All atoms are colored corresponding to their CLS. Black bars denote calculated CLS. To facilitate comparisons with experimental data, a convolution of the CLS with a 0.05 eV Gaussian is shown.