Supporting Information

Insighting the nonlinear optical (NLO) response of pure Aum (2 ≥ m ≤ 7) and copper doped Aum-xCux clusters

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Table S1. Comparison of shapes, theoretical and experimental bond length of pure gold and copper clusters.

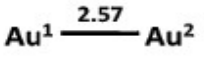
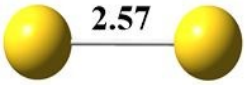
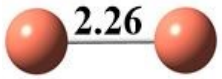
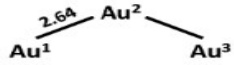
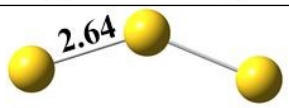
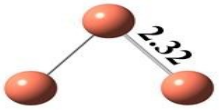
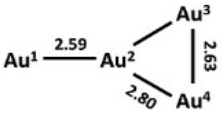
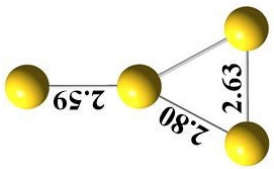
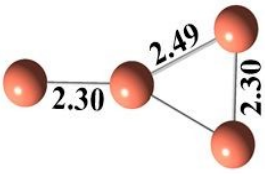
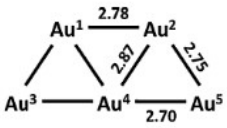
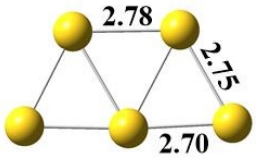
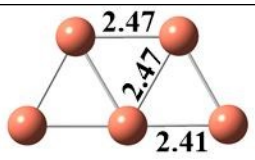
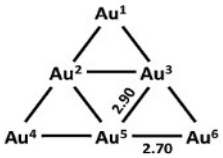
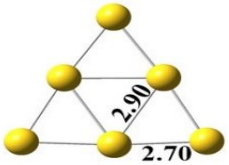
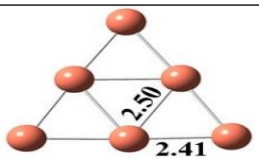
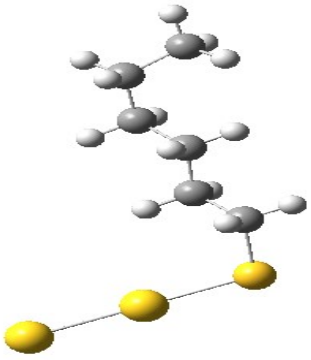
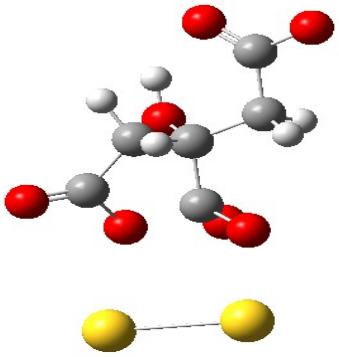
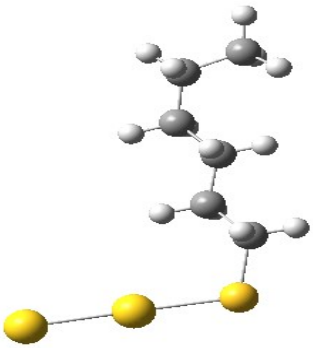
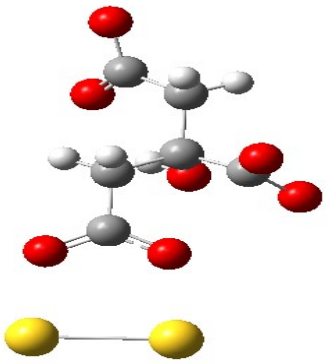
Gold Clusters	B3LYP/LanL2DZ [1]	CAM-B3LYP/LanL2DZ (Calculated)	Gold Experimental bond length [Ref.?]	Copper Clusters	Copper Experimental bond length
Au2			**2.47Å [2]**		**2.22Å [3]**
Au3					
Au4					
Au5					
Au6					

Table S2. Comparison of Polarizability (α) and Hyper Polarizability (β) of pure, thiol and citrate coated Au2 clusters.

Pure Gold Au2	Gold Au2-Thiol	Gold Au2-Citrate
(α)=78.86 **(β)=11.45**	 **(α)=171.74** **(β)=2015.73**	 **(α)= 176.75** **(β)= 834.46**
	 **(α)=174.76** **(β)=6930.75**	 **(α)= 155.16** **(β)= 1354.17**

1. A. Y. Rogachev, X.-D. Wen and R. Hoffmann, *Journal of the American Chemical Society*, 2012, **134**, 8062-8065.
2. J. L. Jules and J. R. Lombardi, *The Journal of Physical Chemistry A*, 2003, **107**, 1268-1273.
3. D. G. Leopold, J. Ho and W. Lineberger, *The Journal of chemical physics*, 1987, **86**, 1715-1726.