Structural and thermodynamic properties of Au_{2-58} clusters

Yi Dong[a)] Michael Springborg[a)] and Ingolf Warnke[b)]

a) Physical and Theoretical Chemistry, University of Saarland, 66123, Germany
b) Department of Chemistry, University of California, Irvine, CA92697, USA

The geometries and electronic properties of the isolated neutral Au_{2-58} are studied theoretically by a parametrized density-functional tight-binding method combined with genetic algorithms. Various descriptors are used in analyzing the structural and electronic properties. In addition, temperature dependence of the vibrational heat capacities of the optimized clusters will also be presented, to study the low temperature properties of the clusters. We find that the vibrational heat capacity of the Au clusters to be strongly size dependent at low temperature.