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Structural and thermodynamic properties of Au_{2-58} clusters YI DONG, MICHAEL SPRINGBORG, University of Saarland, INGOLF WARNKE, University of California, Irvine — The geometries and electronic properties of the isolated neutral Au_{2-58} are studied theoretically using a parametrized density-functional tight-binding method combined with genetic algorithms. Various descriptors are used in analyzing the structural and electronic properties. In addition, the temperature dependence of the vibrational heat capacities of the optimized clusters will be presented, which allow to study the low temperature properties of the clusters. We find that the vibrational heat capacity of the Au clusters is strongly size dependent in particular at low temperatures.

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