Abstract Submitted
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Unbiased studies on structural and electronic properties of gold clusters with up to 58 atoms YI DONG, MICHAEL SPRINGBORG, INGOLF WARNKE, University of Saarland, Germany — Isolated neutral Au_N clusters are studied using a parameterized density-functional tight-binding method combined with genetic algorithms for N from 2 up to 58. Various descriptors are used in analysing the results, including stability, shape, and similarity functions, as well as radial distances of the atoms and the orbital energies, all as functions of N. Based on a harmonic approximation, also the heat capacity of the Au clusters are studied as a function of temperature.

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