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.

Michael Springborg  
University of Saarland, Germany