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Heat Capacities and Magic Numbers in Metal Clusters MICHAEL SPRINGBORG, VALERI G. GRIGORYAN, DENITSA ALAMANOVA, University of Saarland, Saarbruecken, Germany — Using our own *Aufbau/Abbau* method in performing umbiased structure optimization of isolated M_N clusters (with M being a metal) together with the *Embedded-Atom* method for the calculation of the total energy of a given structure, we have optimized the structure of Ni_N, Cu_N, and Au_N clusters with N up to 150. By analysing the total energy as a function of N particularly stable clusters, corresponding to the so-called magic numbers, are identified. Subsequently, we use the harmonic approximation in calculating the vibrational frequencies for each value of N. These are finally using in calculating the molar vibrational heat capacity $\bar{C}_V$ as a function of temperature T. It is been discussed whether, for a given T, $\bar{C}_V$ shows a dependence on N that correlates with the occurrence of magic numbers. An explanation for the observations is being offered.

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