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Structural and energetic properties of nickel clusters MICHAEL SPRINGBORG, VALERI G. GRIGORYAN, University of Saarland, Saarbruecken, Germany — The four most stable structures of Ni_N clusters with N from 2 to 150 have been determined using a combination of the embedded-atom method in the version of Daw, Baskes and Foiles, the *variable metric/quasi-Newton* method, and our own *Aufbau/Abbau* method. A systematic study of energetics, structure, growth, and stability of also larger clusters has been carried through without more or less severe assumptions on the initial geometries in the structure optimization, on the symmetry, or on bond lengths. We present and apply different analytical tools in studying structural and energetic properties of such a large class of clusters. These include means for identifying the overall shape, the occurrence of atomic shells, the similarity of the clusters with, e.g., fragments of the *fcc* crystal or of a large icosahedral cluster, and a way of analysing whether the N-atom cluster can be considered constructed from the $(N-1)$-atom one by adding an extra atom. In addition, we compare in detail with results from chemical-probe experiment. Maybe the most central result is that first for clusters with N above 80 general trends can be identified.

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