Magic structures of binary metallic clusters
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The structure of binary metallic clusters is investigated by a variety of computational tools, ranging from genetic and basin-hopping global optimization algorithms, to molecular dynamics, and to density-functional calculations. Three different binary systems are investigated: Ag-Cu, Ag-Ni, and Ag-Pd. A new family of magic cluster structures is found. These clusters have the common feature of presenting a perfect core-shell chemical arrangement (with an outer Ag shell of monoatomic thickness) and of being polyicosahedra, that is being made of interpenetrating icosahedra of 13 atoms. Core-shell polyicosahedra are of special stability, which originates from the interplay of different factors. First of all, polyicosahedra are very compact structures, so that they maximize the number of nearest-neighbor bonds for a given size. However, in single-element clusters, these bonds are not optimal, since inner bonds are strongly compressed and surface bonds are expanded. This is the contrary of what is required from the bond order - bond length correlation in metals, which favors contracted surface bonds. In binary clusters, the situation is different. Substituting the inner atoms of a single-element polyicosahedron with different atoms of smaller size, the bonds can relax close to their optimal distance. This leads naturally to the appearance of core-shell polyicosahedra. In Ag-Cu, Ag-Ni and Ag-Pd the formation of these structures is reinforced by the tendency of Ag atoms to surface segregation. A similar mechanism of structural relaxation, originating from the interplay of cluster geometry and bond order - bond length correlation, is also the cause of the destabilization of icosahedral structures in pure Pt and Au clusters. In these clusters, the compressed inner atoms of the icosahedra can relax because of the formation of rosette structures at vertices in the outer layer.