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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.