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Global optimization of free and supported metallic nanoclusters GIULIA ROSSI, Dipartimento di Fisica, Universita' di Genova, FRANCESCA BALETTO, ICTP, Trieste, Italy, CHRISTINE MOTTET, CRMCN/CNRS, Marseille, France, ARNALDO RAPALLO, ISMAC/CNR, Milano, Italy, RICCARDO FERRANDO, Dipartimento di Fisica, Universita' di Genova, Italy — The global optimization of free and supported metallic nanoclusters is performed by two different approaches: a genetic algorithm and a basin-hopping algorithm. Optimization has been applied to a series of different systems, such as free pure clusters (Pd, Ag, Cu, Ni), free binary clusters (AgPd, AgCu, AgNi) and supported Pd clusters on MgO(100) substrates. The metals are described by a many-body potential derived within a tight-binding scheme in the second moment approximation, while the interaction between the metallic atoms and the oxide is modeled by an analytical potential fitted to *ab initio* calculations. As regards free hetero-metallic clusters, the optimization has led to the location of a family of stable core-shell polyicosahedral structures. According to this geometrical configuration, clusters structures are made of several interpenetrating icosahedra, and the atoms with smaller radius (Cu, Ni, Pd) occupy volume sites while Ag atoms are placed on the cluster surface. Such a geometrical configuration agrees with the bond order-bond length correlation, that is typical of metallic interactions. Concerning supported Pd clusters, their structure modifications resulting from the interaction with the substrate are investigated as a function of clusters size.

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