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Density functional investigation of silver, palladium and silver-palladium small sized clusters
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Abstract

We have investigated the geometrical and electronic properties of small sized Ag and Pd as well as bimetallic Ag-Pd clusters. By means of a pseudopotential scheme within density functional theory, we found the ground-state geometries and the spin multiplicity state for this family of metallic clusters. We computed the binding energy and the atom addition energy change for these family of clusters with two different density functionals. Ag and Pd cluster series exhibit a clear different behavior as a consequence of the atomic electronic structure. In particular we discuss the high symmetry silver clusters and the trends in the small sized bimetallic Ag-Pd systems.

Keywords

Silver, palladium and silver-palladium clusters, electronic structure.