DFT Optimization of Symmetric Be$_2$Si Cage Clusters

ROBERT BINNING, DANIEL BACELO, Universidad Metropolitana, San Juan, PR 00928-1150 — Density functional theory calculations have been performed on several beryllium silicide cage clusters in which the atoms occupy the vertices of classic Archimedean solids. The BPW91 functionals with numerical basis sets were employed in the optimizations. The calculations were carried out to confirm the hypothesis that stable Be$_2$Si clusters may be obtained by substituting Si for Be atoms in stable pure beryllium clusters. Stable beryllium clusters are obtained from symmetrical Be$_n$ polyhedra in which sides are triangular or capped pentagonal, and the Archimedean clusters composed of these elements with Si substitutions are indeed found to produce stable beryllium silicides.