DFT Optimization of Symmetric Be$_2$Si Cage Clusters ROBERT
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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 em-
ployed in the optimizations. The calculations were carried out to confirm the hy-
pothesis 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 sym-
metrical 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.

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