Study of the Si_{45} cluster

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Abstract

There are a lot of works published on Si_{45} cluster and it is shown that the structure of the Si_{45} cluster is constructed by a fullerene-like cage surrounding a core of some Silicon atoms.

In our work we propose a structure for the Si_{45} cluster which is constructed by a Si_{38} fulerene-like cage encapsulating a core of seven Silicon atoms inside the cage. Six of the core atoms are arranged in such a way so as each one of them to be placed over the center of non-neighbouring faces of the fullerene-like cage. The seventh core atom is placed in the center of the cluster. As there are only six non-neigbouring faces of the Si_{38} fulerene-like cage, (for every one of the 17 isomers of a 38-atom fullerene), the saturation of the dangling bonds is succeeded at the most efficient way and as a result this structure is found to be the most stable one.