Study of the Si_{38} fullerene-like cages

Zacharias G. Fthenakis[a,b],George Froudakis[c], Remco Havenith[d], Madhu Menon[e,f], Patric W. Fowler[d],Antonios N. Andriotis[a]

[a] *Institute of Electronic Structure and Laser, P.O. Box 1527, Heraklion-Crete 71110, Greece*

[b] *Dept of Physics, University of Crete, Heraklion-Crete, 71110, Greece*

[c] *Dept of Chemistry, University of Crete, Heraklion-Crete, 71110, Greece*

[d] *Dept of Chemistry, University of Exeter, Stocker Road, Exeter, UK EX4 4QD*

[e] *Dept of Physics and Astronomy, Univ. of Kentucky, Lexington, KY40506-0055*

[f] *Center for Computational Sciences, Univ. of Kentucky, Lexington, KY40506-0055*

Abstract

Knowing that Silicon is contiguous to Carbon on the periodic table and following the extensive search on Carbon fullerenes, the natural question that arises is : "What about Silicon fullerenes ?".

In this work we try to give an answer to this question, finding the optimum structures of 17 isomers of the Si_{38} fullerene-like cage-clusters. We apply a Tight Binding Molecular Dynamics (TBMD) technique in order to make a fast search in the configuration space for the energeticaly optimum structures. Within this TBMD method, 17 geometrical (cage-like) structures (one for each isomer) are proposed as the structures with the lowest energy. These results were verified by more accurate computational schemes. In particular, for each one of these structures three more accurate but more time consuming calculations were carried out, namely, a non Orthogonal Tight Binding, a DFT and a RHF calculation. The results of these calculations were found in a very good agreement with the results obtained with the initially applied TBMD method.