Assembling small silicon clusters using criteria of maximum matching of the Fukui functions

Osorio, Edison

Ferraro, Marta B.

Oña, Ofelia B.

Cardenas, Carlos

Fuentealba, Patricio

Tiznado, William

In this work, we present a methodology inspired by criteria of "maximum matching" between the Fukui functions to predict the best interaction between small silicon clusters to form larger ones. The model is based on the topological analysis of the Fukui functions. We tested the methodology in the formation of Si4-Si8 using a set of small Si2-Si6 clusters as building blocks in ground state structures in singlet and triplet multiplicities. In all of the cases, the Fukui function predicts the formation of the large cluster in its ground state structure, but the number of reaction channels increases with the cluster size. © 2011 American Chemical Society.