

Supporting Information

Low-Energy Structures and Electronic Properties of Large-Sized Si_N Clusters ($N = 60, 80, 100, 120, 150, 170$)

Di Wu,^{†,‡} Xue Wu,[†] Xiaoqing Liang,[†] Ruili Shi,[†] Zhe Li,[†] Xiaoming Huang,[§] Jijun Zhao^{*,†}

[†]Key Laboratory of Materials Modification by Laser, Ion and Electron Beams (Dalian University of Technology), Ministry of Education, Dalian 116024, China

[‡]School of Science, Shenyang Aerospace University, Shenyang 110136, China

[§]School of Ocean Science and Technology, Dalian University of Technology, Panjin 124221, China

* Corresponding author. E-mail : zhaojj@dlut.edu.cn

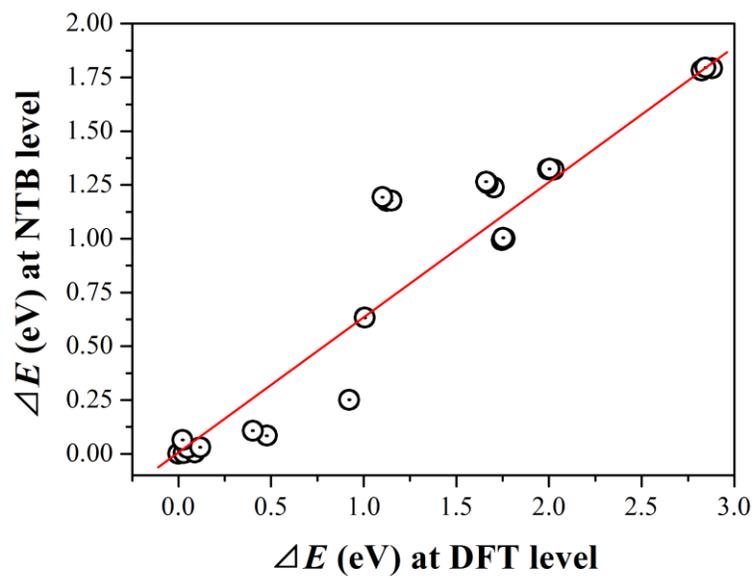


Figure S1. Relative energies ΔE from NTB model versus ΔE from DFT single-point energies for 25 selected isomers of Si_{60} .

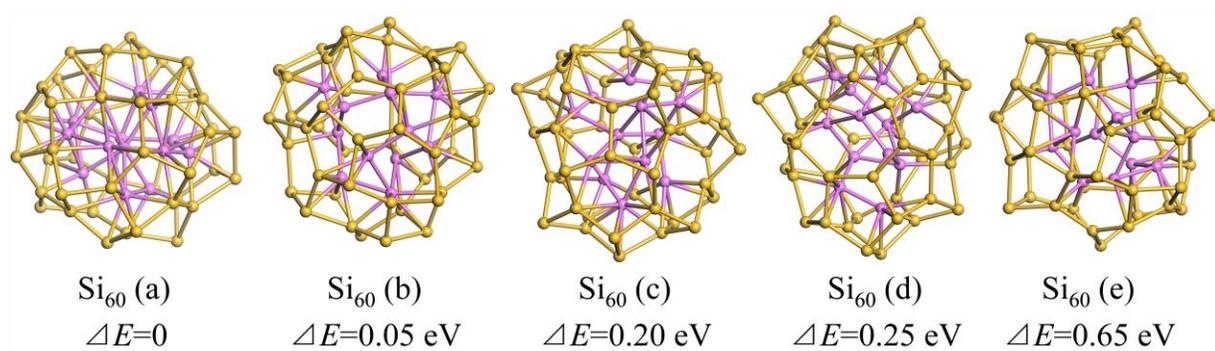


Figure S2. Structures and relative energies (ΔE) for isomers of Si₆₀ from five independent BH search. The core atoms are highlighted in pink color and the atoms on outer cage are in yellow.

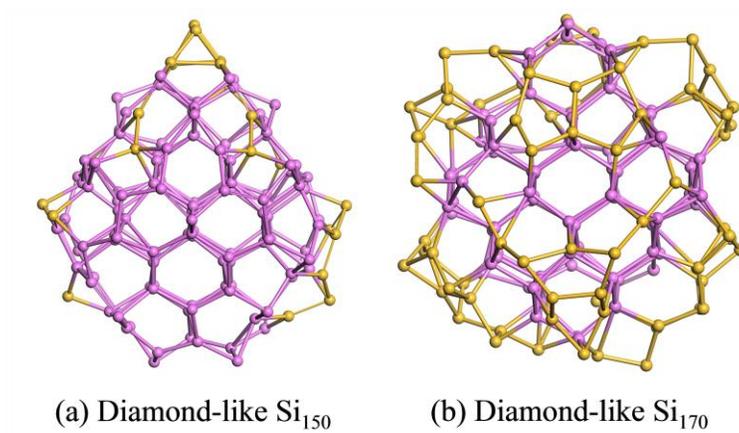


Figure S3. Low-energy diamond-like structures of Si_{150} and Si_{170} clusters. The majority atoms in diamond-like core structure are in pink, while the rest of surface atoms are in yellow.