

## Supporting Information

### Low-Energy Structures and Electronic Properties of Large-Sized $\text{Si}_N$ Clusters ( $N = 60, 80, 100, 120, 150, 170$ )

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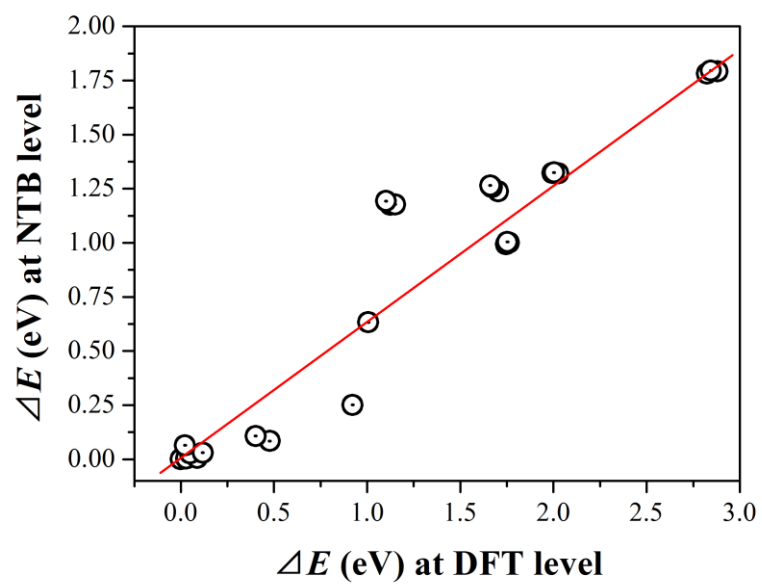
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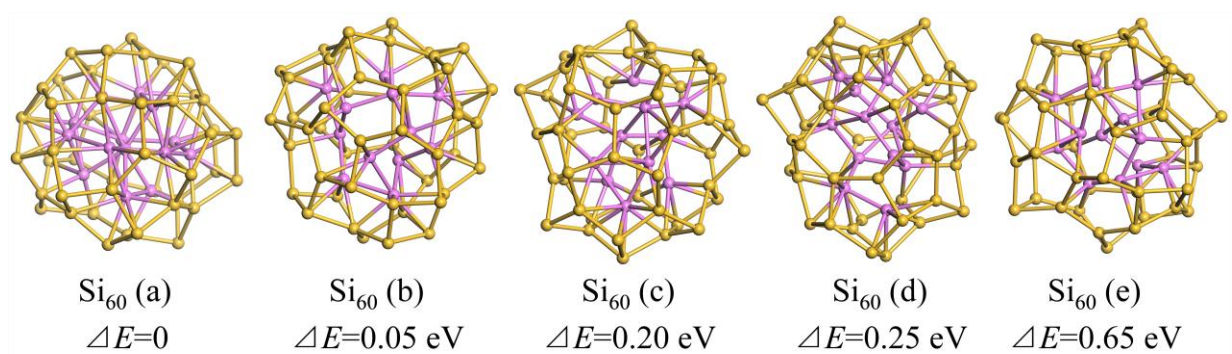
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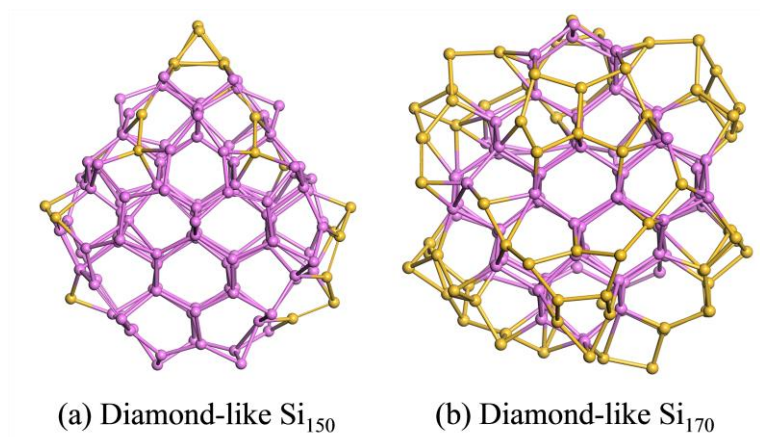
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**Figure S1.** Relative energies  $\Delta E$  from NTB model versus  $\Delta E$  from DFT single-point energies for 25 selected isomers of  $\text{Si}_{60}$ .



**Figure S2.** Structures and relative energies ( $\Delta E$ ) for isomers of  $\text{Si}_{60}$  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<sub>150</sub> and Si<sub>170</sub> clusters. The majority atoms in diamond-like core structure are in pink, while the rest of surface atoms are in yellow.