

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Dimer and NEB studies on Si I_4 chain and the ground state I_4 ¹

YAOJUN DU, JOHN WILKINS, Ohio State University — The dimer method explores the energy landscape of two important Si four-interstitials: 1) the ground state and 2) chain extending in the [110] direction. DFT-GGA calculations find the ground state is an extremely stable with 3.3-8.4 eV barrier to five dimer-identified neighboring minima. Those minima are 0.9-1.8 eV above the ground state. In contrast, the chain's most accessible local minimum has 1 eV barrier to the three-interstitial ground state plus a nearby single interstitial with a tiny 0.1 eV barrier to form chain. The tight-binding, nudged-elastic-band pathway from the chain to the four-interstitial ground state has two structurally close local minima with a separation of 4.4 Å. The chain-to-ground-state barrier is 1.4 eV, suggesting that the tri-interstitial could grab an interstitial to form a four-interstitial chain that could grow into a longer chain without falling into the four interstitial ground state.

¹This work was supported in part by DOE-Basic Energy Sciences, Division of Materials Sciences (DE-FG02-99ER45795)

Yaojun Du
Ohio State University

Date submitted: 19 Nov 2004

Electronic form version 1.4