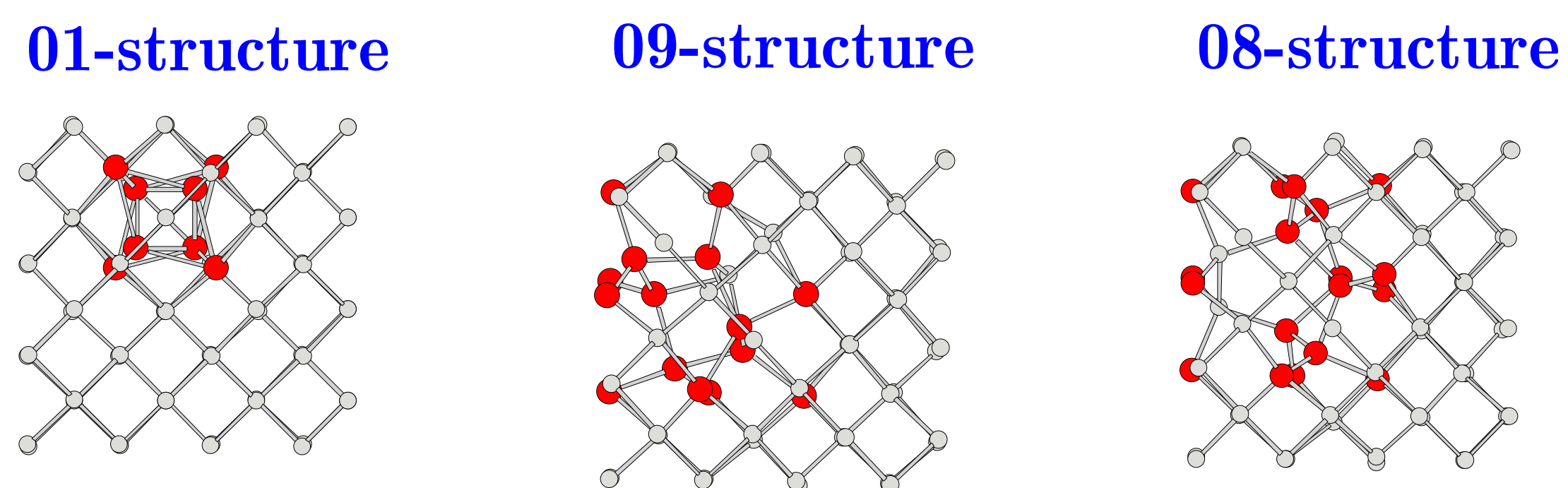


# From point defect to interstitial chain in Si and fast diffusion mechanism of Si tri-interstitial

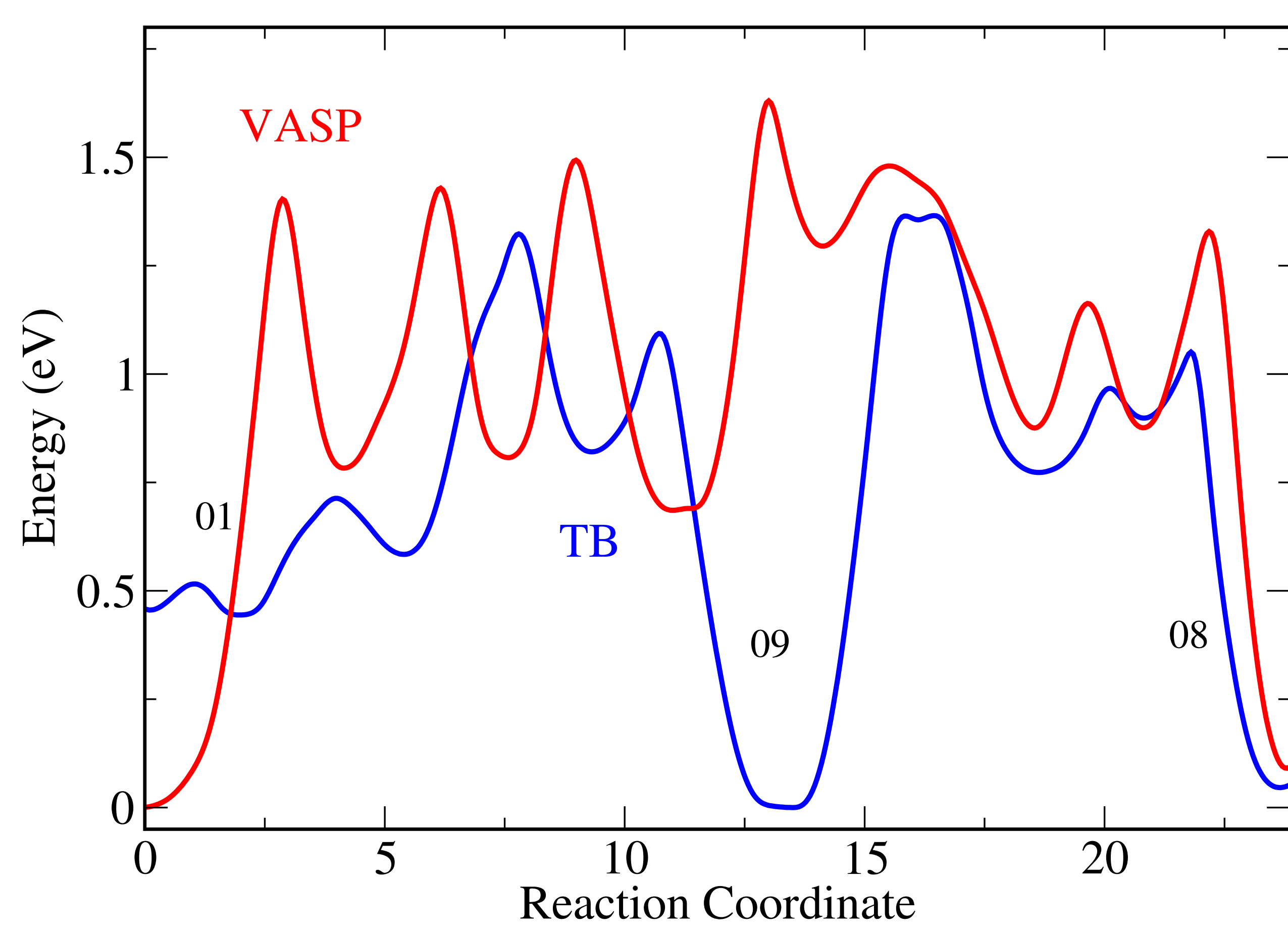
Y. A. DU and J. W. Wilkins

## Three lowest-lying defect structures



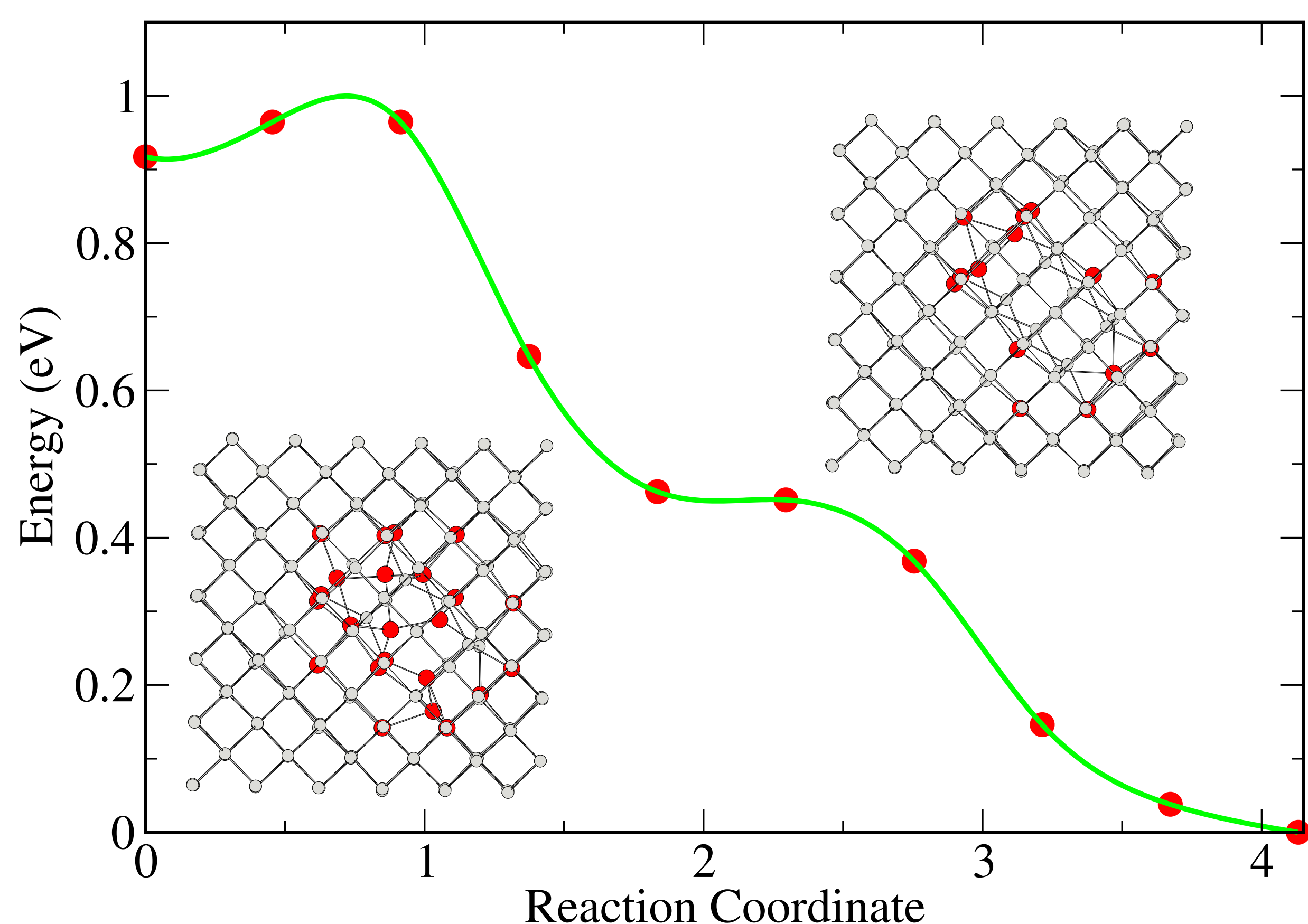
- The submicroscopic Si-interstitials are believed to transiently enhance boron diffusion<sup>1</sup> in boron-implanted silicon wafer. We perform simulations on silicon tri-interstitials.
- Three lowest-lying structures in 67-atom bulk appear in time sequence during the MD simulation with Lenosky tight binding potential<sup>2</sup> at 800 K. Defect atoms are marked by red.

## Pathway connecting 01, 09 and 08

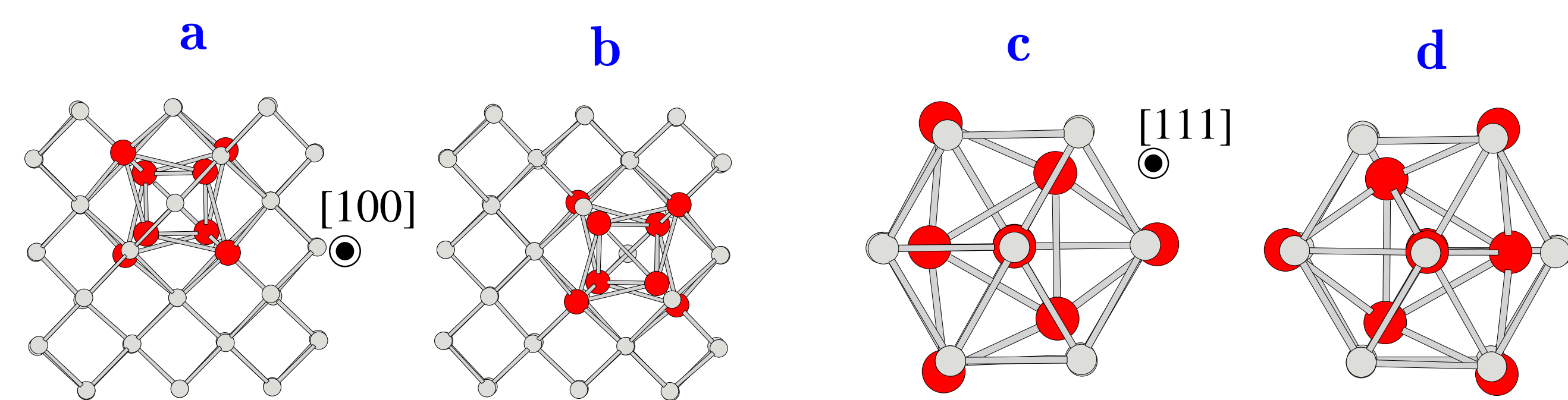


- Extensive explorations with the dimer searching<sup>3</sup> scheme on the three lowest-lying defect structures reasonably exclude the existence of other low-lying defect structures surrounding them.
- Using both **Lenosky tight binding potential** and **ab-initio calculations**, the nudged-elastic-band method<sup>4</sup> reveals the pathways connecting the three lowest-lying structures
- Vienna Ab-initio Simulation Package with NEB
  - Plane wave basis and ultrasoft pseudopotentials
  - $E_{\text{cut}} = 250 \text{ eV}$  and  $3 \times 3 \times 3$  k-point mesh

## The extend tri-interstitial develops a four-interstitial chain by capturing a single interstitial

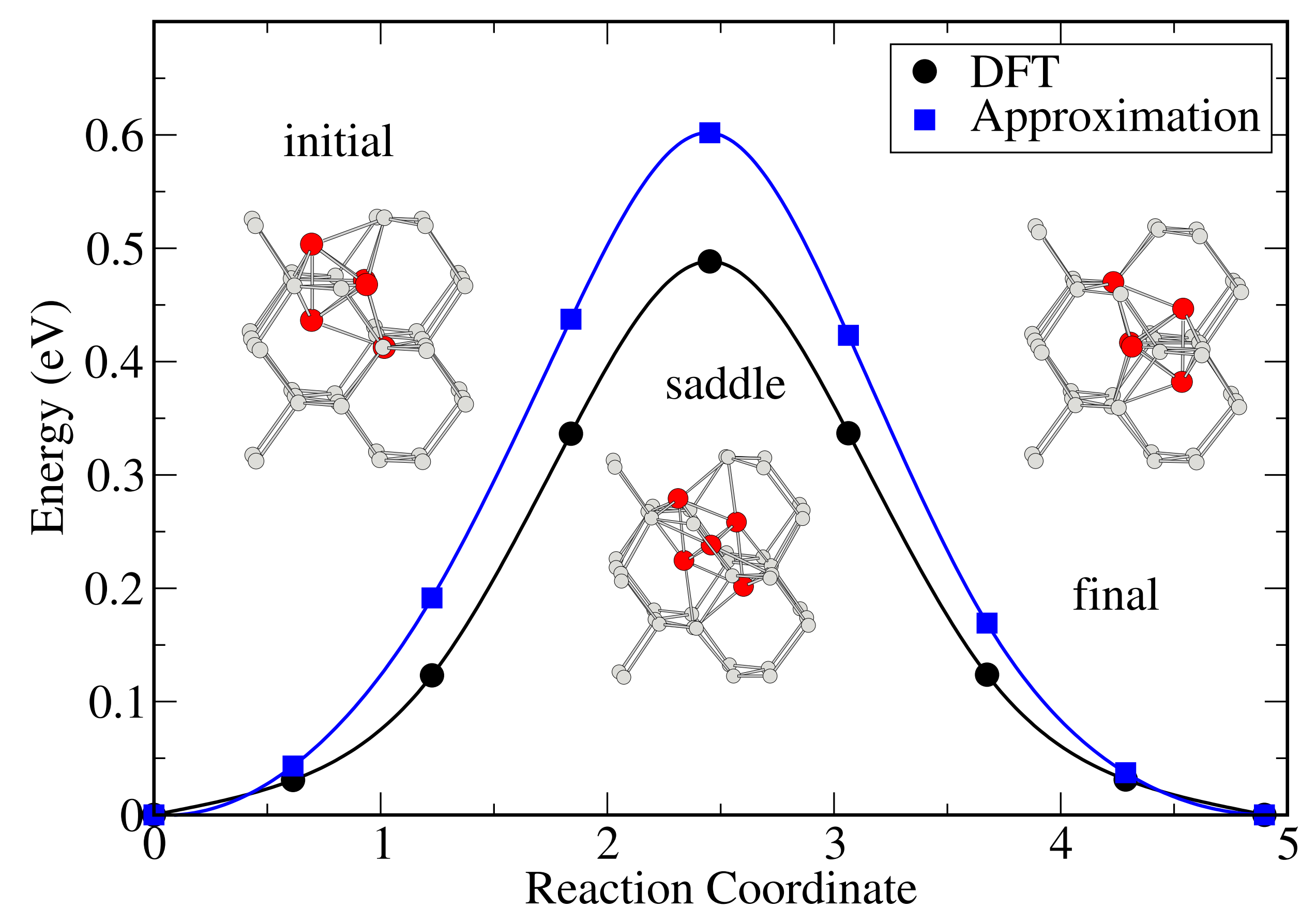


## Self-diffusion of compact tri-interstitial

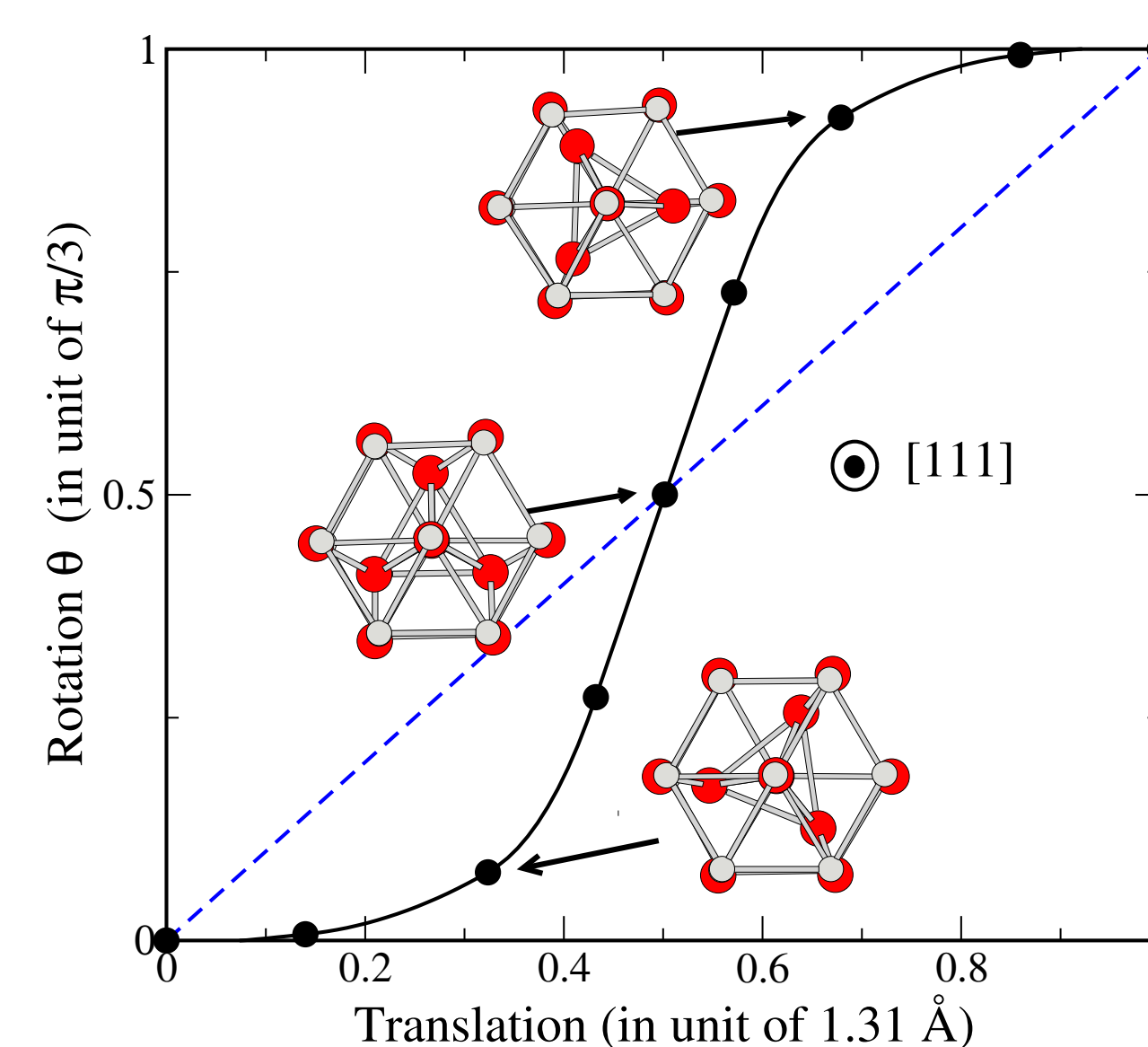


- (a) and (b) are the initial and final state viewed from [100] direction, (c) and (d) are the initial and final state viewed from [111] direction.

## Pathway for 01 to 01 self-diffusion



## collective motion of five atoms



- Self-diffusion pathway of compact tri-interstitial by VASP estimates the transition rate  $\Gamma = 1.9 \text{ THz } e^{-2.1} \exp(-0.48/k_B T)$ .
- The self-diffusion is well described by the translate of rotation of five atoms that form a double-tetrahedron.
- The compact tri-interstitial hops into four neighbouring sites following the four possible bond directions, resulting a diffusion constant  $D = 0.2 \cdot 10^{-5} \exp(-0.48 \text{ eV}/k_B T) \text{ cm}^2/\text{s}$  compared to the experimental result<sup>5</sup> of  $\sim 10^{-5} \exp(-0.40 \text{ eV}/k_B T) \text{ cm}^2/\text{s}$ .

## Conclusion

- The pathway connecting 01, 09 and 08-structures has been revealed using VASP-DFT and TB potential. The extended tri-interstitial develop to a interstitial chain by capturing a single interstitial.
- The compact tri-interstitial is a mobile structure that serves a significant contributor to the self-diffusion of Si interstitials.

## Acknowledgement

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