

Abstract Submitted
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Computational studies of thermal evolutions of extended interstitial defects in silicon.¹ HYOUNGKI PARK, JOHN W. WILKINS, The Ohio State University — Annealing induces the nucleation of extended defect clusters in silicon and their evolution, where clusters grow by capturing or interchanging interstitials, and change their crystallographic structure in order to minimize the formation energy. Extensive molecular dynamics (MD) simulations and first-principle nudged elastic band (NEB) simulations explore the thermal transitions from one structure to another of three energetically competing extended interstitial defects: two rod-like defects $\{311\}$ and $\{111\}$, and Frank dislocation loop. MD simulations capture critical sequences of atomistic processes during transitions from $\{311\}$ and $\{111\}$ defects to Frank loops as their atomic configurations and habit planes change, and massively parallelized NEB simulations within the local density approximation reveal the energetics of reaction barriers.

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