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Relative stability of extended interstitial defects in silicon: large-scale classical MD and first-principles DFT.[1] HYOUNGKI PARK, JOHN WILKINS, The Ohio State University — Extensive simulations for defected Si reveal the relative thermal and temporal stability of extended interstitial defects: 311 and 111 rod-like defects, and Frank dislocation loops. Classical molecular dynamics simulations provide the atomic configurations of those defects, and show that the energetically favored structures change from 311 rod-like defects to Frank loops as the number of interstitals increases, which is consistents with the experimentally-observed transition from rod-like defects to Frank loops after long, high-temperature annealing processes [1,2]. This relative stability is validated with massively parallelized density-functional calculations of 1500-atoms 2D supercells. Relaxation of experimentally-observed-size defect cluster demonstrates the energetic hierarchy is dependent on the number of interstitials in the defect clusters. [1] L. S. Robertson et al., J. Appl. Phys. 87, 2910 (2000). [2] G. Z. Pan et al., J. Non-Crystalline Solids 352, 2506 (2006).

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