

Supplementary information

A list of supplementary information for the manuscript titled “A topological point defect regulates the evolution of extended defects in irradiated silicon.”

1. A table of the formation energy per interstitial and band gaps from DFT calculations with HSE and PBE exchange-correlation functionals for extended interstitial defects modeled infinitely long along $\langle 011 \rangle$.
2. A schematic illustration of a transition path from a $\{311\}$ *EIIIOIE* defect to a Frank loop with an eight-member ring.
3. A schematic illustration of a transition path from a $\{311\}$ *EIOIOIE* defect to a Frank loop with two eight-member rings (or the $\{111\}$ defect).
4. A graph of calculated barriers at each step of a transition path from a $\{311\}$ to a Frank loop.

TABLE I. Summary of the formation energies per interstitial E_f and band gaps E_g for infinitely long $\{311\}$, $\{111\}$ defects, and Frank dislocation loops with various numbers of interstitial chains listed in the second column. For $\{311\}$ defects with eight-member rings O_s , the sequence of interstitial chains and eight-member rings along $[2\bar{3}\bar{3}]$ on $\{311\}$ is shown explicitly since different arrangements produce different energies. Infinite planar defects, i.e., defects with infinite number of interstitial chains, are denoted by the sequence of periodic unit in $//$, e.g., $/IO/$ represents $\dots IOIOIOIOIO \dots$.

Structure	No. of interstitial chains	E_f (eV)		E_g (eV)		
		HSE	PBE	HSE	PBE	
$\{311\}$ defect	Bulk	0	0.00	0.00	1.15	0.58
	1	1.24	1.38	1.04	0.47	
	2	1.10	1.14	0.97	0.40	
	4	1.03	1.07	0.72	0.21	
	6	1.01	1.07	0.43	0.00	
	IOI	1.26	1.25	1.02	0.46	
	$IOII$	1.08	1.10	0.96	0.42	
	$IIOII$	1.00	1.03	0.96	0.40	
	$/I/$	0.93	1.07	0.11	0.00	
$/IO/$	0.92	1.12	1.03	0.45		
$/IIO/$	0.70	0.90	0.97	0.41		
$/IIIO/$	0.72	0.91	0.94	0.37		
$\{111\}$ defect	4	1.14	1.24	0.86	0.32	
	∞	0.73	0.94	0.98	0.41	
Frank loops	4	1.44	1.51	0.35	0.00	
	5	1.34	1.40	0.34	0.00	
	6	1.27	1.33	0.32	0.00	
	7	1.21	1.27	0.32	0.00	

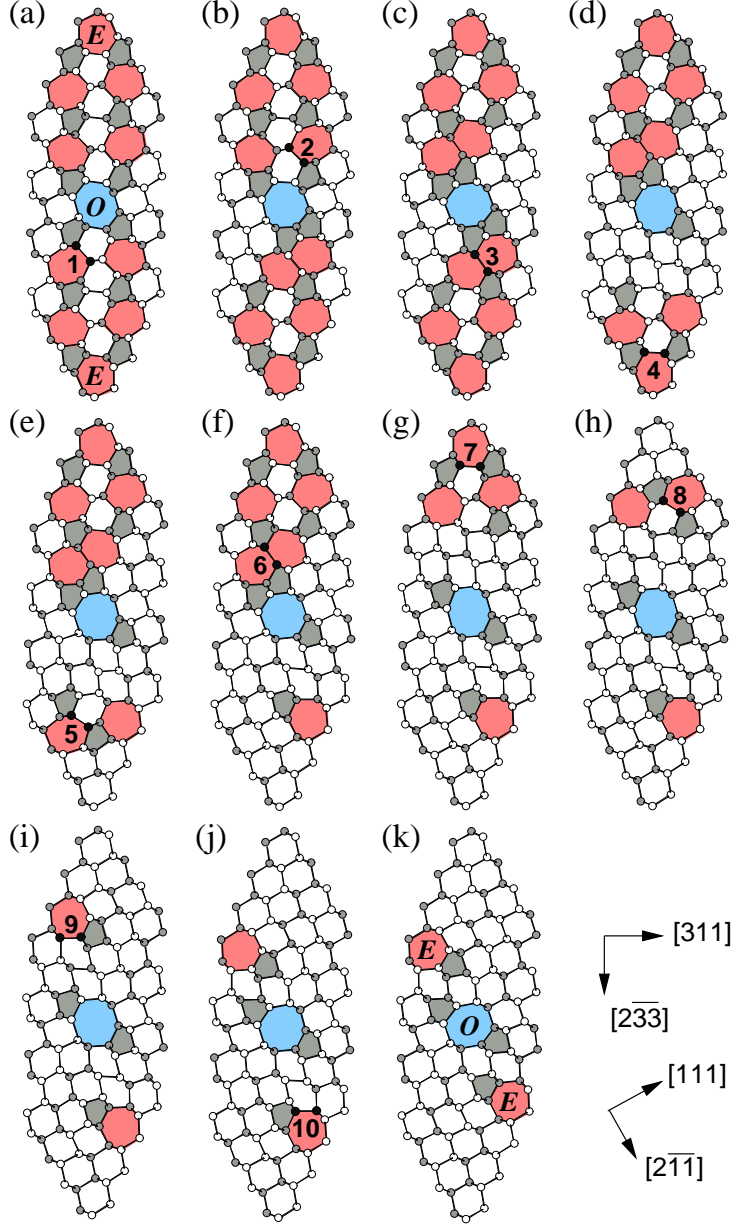


FIG. 1. Transformation from a $\{311\}$ *EIIIOIE* defect to a Frank loop with an eight-member ring, from (a) to (i). Rotations of pairs of atoms in seven-member rings in the $\{311\}$ defect convert five- and seven-member rings to six-member rings and induce the transformation to the Frank loop. The essential number of rotations of pairs to complete the transformation from a $\{311\}$ defect to a Frank loop is same as the number of interstitial atoms. Steps from (i) to (k) are not really part of the transformation, but are extra steps making the Frank loop more stable by aligning two end-units. In each figure, five-, seven-, and eight-member rings are shaded in gray, pink, and light blue, respectively. Rotating atoms are colored black, and sequentially indexed by evolution stages.

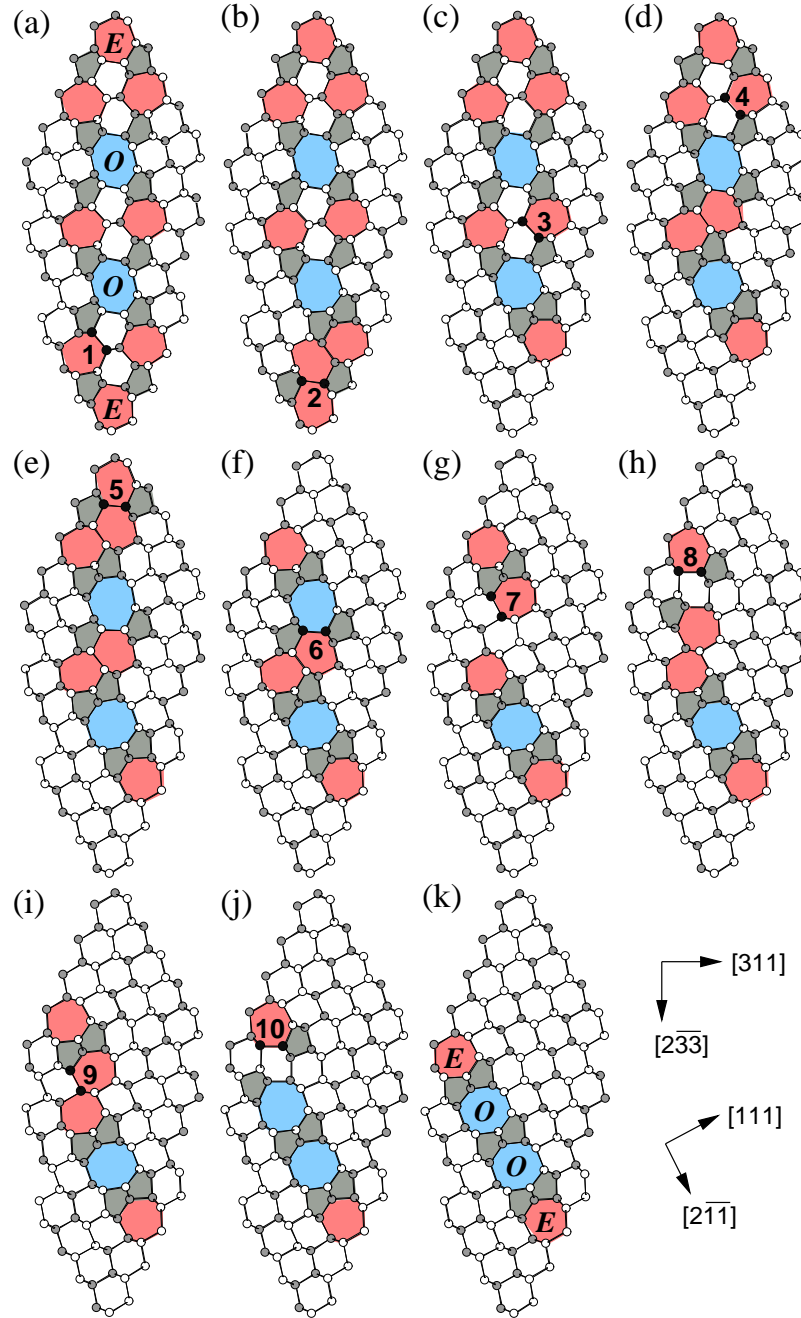


FIG. 2. Transformation from a $\{311\}$ $EIOIOIE$ defect to a Frank loop with two eight-member rings, from (a) to (g). Similar to Fig. 1, (g)–(k) are extra steps making the the Frank loop more stable by aligning two end-units. The Frank loop of (k) has the same structure as the proposed $\{111\}$ defect.

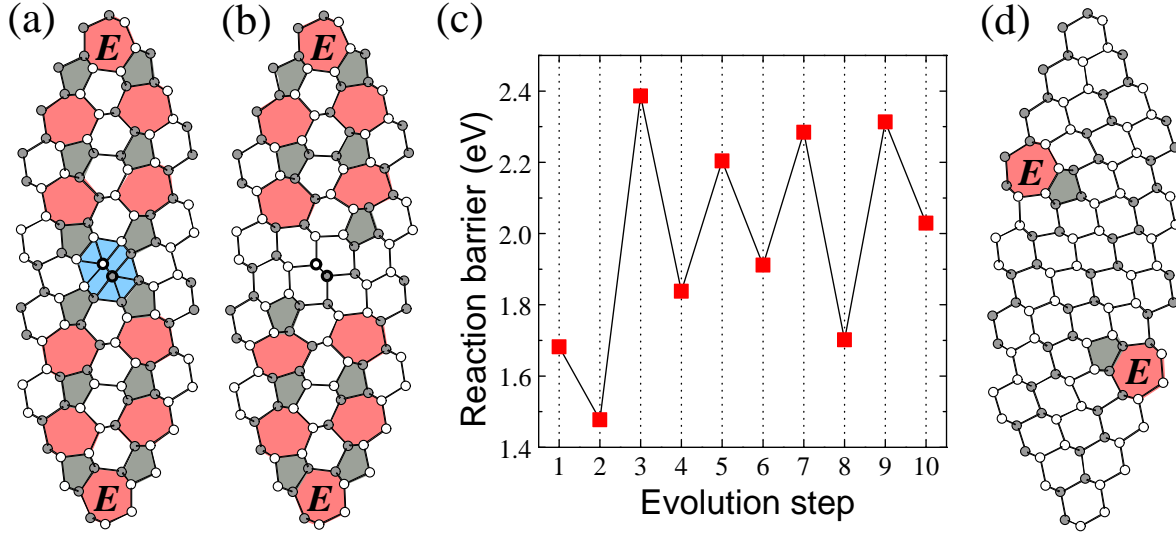


FIG. 3. Calculated barriers of the rotating pairs that transform from the structure of “a $\{311\}$ $EIIIOIE$ defect + an additional di-interstitial” to a Frank loop. A di-interstitial, atoms in bold circles, fills the eight-member ring of the $\{311\}$ $EIIIOIE$ defect in (a), and the structure relaxes to be (b). The graph of (c) shows barriers at each step of evolution stages from structure (b) to (c) following the same transition path illustrated in Figure 1. Barriers for rotating pairs in seven-member rings are about 1.5 – 2.4 eV depending on the evolution stages and local structures.