Supporting information

Point Defects in Lines in Single Crystalline Phosphorene:

Directional Migration and Tunable Band Gaps

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Content:

Figure S1. The optimized structures of phosphorene with point defects.

Figure S2. The MEP of SV1 defect migrating along armchair or zigzag direction.

Figure S3. The calculated band structure and DOS of the perfective phosphorene.

Figure S4. The calculated DOS and partial DOS projected on the phosphorous atoms in the defective region for phosphorene containing line defects.

Figure S5. Line defects along T direction.

Figure S6. The charge distribution of defective states in phosphorene containing SV1 line defect.

Figure S7. Electronic band structures of phosphorene with line defects

Table S1. The average formation energies of extended line defects



Figure S1. The optimized structure of SV1 defect when migrating along (a) zigzag and (b) armchair direction.



Figure S2. The calculated MEP of SV defect migrating along (a) zigzag and (b) armchair direction.



Figure S3. The calculated (a) electronic band structure and (b) total DOS of the perfect phosphorene.



Figure S4. Total and projected DOS on phosphorous atoms in defective region are plotted for phosphorene containing (a) SW1-Z, (b) SW1-A, (c) SW2-Z, (d) SW2-A, (e) SV1-Z, (f) SV1-A, (g) SV2-Z, (h) SV2-A, (i) DV1-Z, (j) DV1-A, (k) DV2-Z, or (l) DV2-A line defect. The projected DOS are plotted with red lines and total DOS are plotted with black line.



Figure S5. Line defects along T direction. The defective region is labelled with red dotted lines. (a) SW1-T, (b) SW2-T, (c) SV1-T, (d) SV2-T, (e) DV1-T, and (f) DV2-T.



Figure S6. The calculated charge density distribution of defective states crossing the Fermi energy level of phosphorene with (a) SV1-Z or (b) SV1-A line defect, respectively. The isosurface value is 0.002 e/bohr³.



Figure S7. Electronic band structures of phosphorene with (a) SW1-T, (b) SW2-T, (c) SV1-T, (d) SV2-T, (e) DV1-T, and (f) DV2-T line defect, respectively. The fermi level is marked by dotted lines and set to zero.

Table S1. The average formation energies of extended line defects (E_f^{LD} in unit of eV/cell, and $E_{f/l}^{LD}$ in unit of eV/Å), the band gaps of phosphorene containing line defects (E_G in unit of eV), and formation energies of point defect (E_f^{PD} in unit of eV) are summarized.

	E_{f}^{LD} (eV)	$E_{f/l}^{LD}$ (eV [·] Å ⁻¹)	E _G (eV)	E_{f}^{PD} (eV)
SW1-T	0.888	0.161	0.902	1.331
SW2-T	0.768	0.132	1.204	1.015
SV1-T	1.509	0.264	Metal	1.633
SV2-T	2.067	0.366	Metal	2.033
DV1-T	1.537	0.280	0.589	1.919
DV2-T	1.417	0.256	0.877	3.046