Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Properties of diamane anchored with different groups

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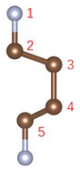
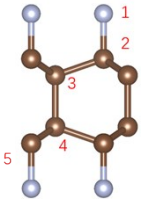
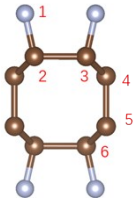
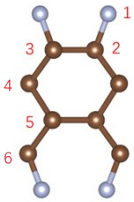
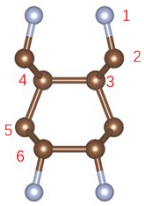
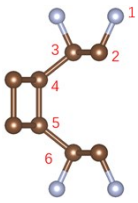
Table S1 Bond lengths are given in Å for the different phases decorated by five types of the functional group.

Configurations·	H	F	OH	Cl	NH_2
 chair1	d_{12}=1.109 d_{23}=1.538 d_{34}=1.558 h_{23}=0.488 h_{45}=0.488	d_{12}=1.378 d_{23}=1.559 d_{34}=1.552 h_{23}=0.503 h_{45}=0.503	d_{12}=1.422 d_{23}=1.580 d_{34}=1.545 h_{23}=0.414 h_{45}=0.414	d_{12}=1.747 d_{23}=1.670 d_{34}=1.534 h_{23}=0.508 h_{45}=0.508	d_{12}=1.473 d_{23}=1.624 d_{34}=1.536 h_{23}=0.518 h_{45}=0.518
 chair2	d_{12}=1.109 d_{23}=1.536 d_{34}=1.586 h_{23}=0.490 h_{45}=0.491	d_{12}=1.377 d_{23}=1.558 d_{34}=1.570 h_{23}=0.508 h_{45}=0.508	d_{12}=1.425 d_{23}=1.561 d_{34}=1.562 h_{23}=0.520 h_{45}=0.520	d_{12}=1.743 d_{23}=1.668 d_{34}=1.562 h_{23}=0.515 h_{45}=0.516	d_{12}=1.471 d_{23}=1.623 d_{34}=1.559 h_{23}=0.534 h_{45}=0.525
 boat1	d_{12}=1.106 d_{23}=1.563 d_{34}=1.528 d_{45}=1.573 h_{34}=0.631 h_{56}=0.633	d_{12}=1.376 d_{23}=1.630 d_{34}=1.546 d_{45}=1.574 h_{34}=0.620 h_{56}=0.620	d_{12}=1.414 d_{23}=1.706 d_{34}=1.535 d_{45}=1.565 h_{34}=0.622 h_{56}=0.622		d_{12}=1.463 d_{23}=1.789 d_{34}=1.576 d_{45}=1.562 h_{34}=0.633 h_{56}=0.632
 boat2	d_{12}=1.098 d_{23}=1.529 d_{34}=1.539 d_{45}=1.555 h_{34}=1.221 h_{56}=1.221	d_{12}=1.361 d_{23}=1.553 d_{34}=1.545 d_{45}=1.595 h_{34}=1.160 h_{56}=1.160	d_{12}=1.378 d_{23}=1.571 d_{34}=1.607 d_{45}=1.595 h_{34}=0.988 h_{56}=1.153		
 boat3	d_{12}=1.102 d_{23}=1.536 d_{34}=1.581 d_{45}=1.555 h_{23}=0.693 h_{56}=0.693	d_{12}=1.368 d_{23}=1.551 d_{34}=1.640 d_{45}=1.564 h_{34}=0.682 h_{56}=0.681	d_{12}=1.401 d_{23}=1.548 d_{34}=1.722 d_{45}=1.558 h_{34}=0.685 h_{56}=0.685		
 boat4	d_{12}=1.100 d_{23}=1.536 d_{34}=1.519 d_{45}=1.599 h_{34}=1.024 h_{56}=1.024	d_{12}=1.387 d_{23}=1.569 d_{34}=1.533 d_{45}=1.597 h_{34}=0.961 h_{56}=0.961	d_{12}=1.416 d_{23}=1.589 d_{34}=1.546 d_{45}=1.591 h_{34}=0.962 h_{56}=0.962	d_{12}=1.744 d_{23}=1.728 d_{34}=1.601 d_{45}=1.579 h_{34}=0.843 h_{56}=0.843	d_{12}=1.468 d_{23}=1.666 d_{34}=1.575 d_{45}=1.585 h_{34}=0.921 h_{56}=0.932

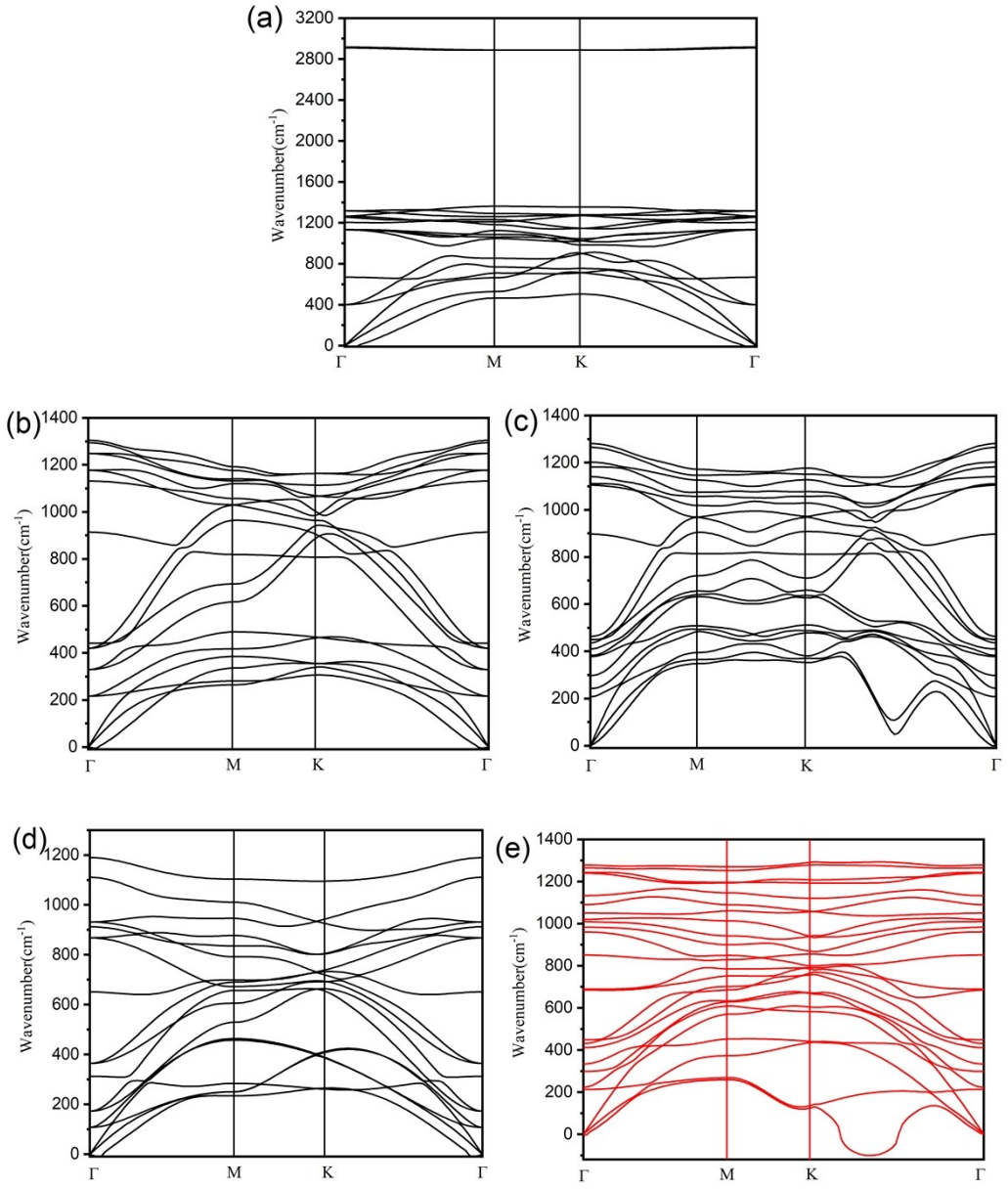
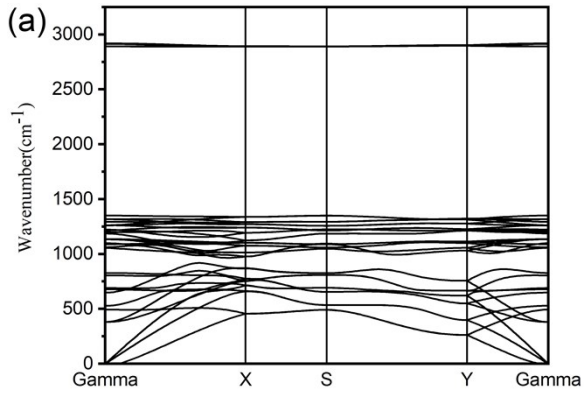


Fig. S1 phonon spectrums: (a) chair1-H (4◊4), (b) chair1-F (4◊4), (c) chair1-OH (3◊3), (d) chair1-Cl (4◊4), (e) chair1-NH_2 (3◊3).



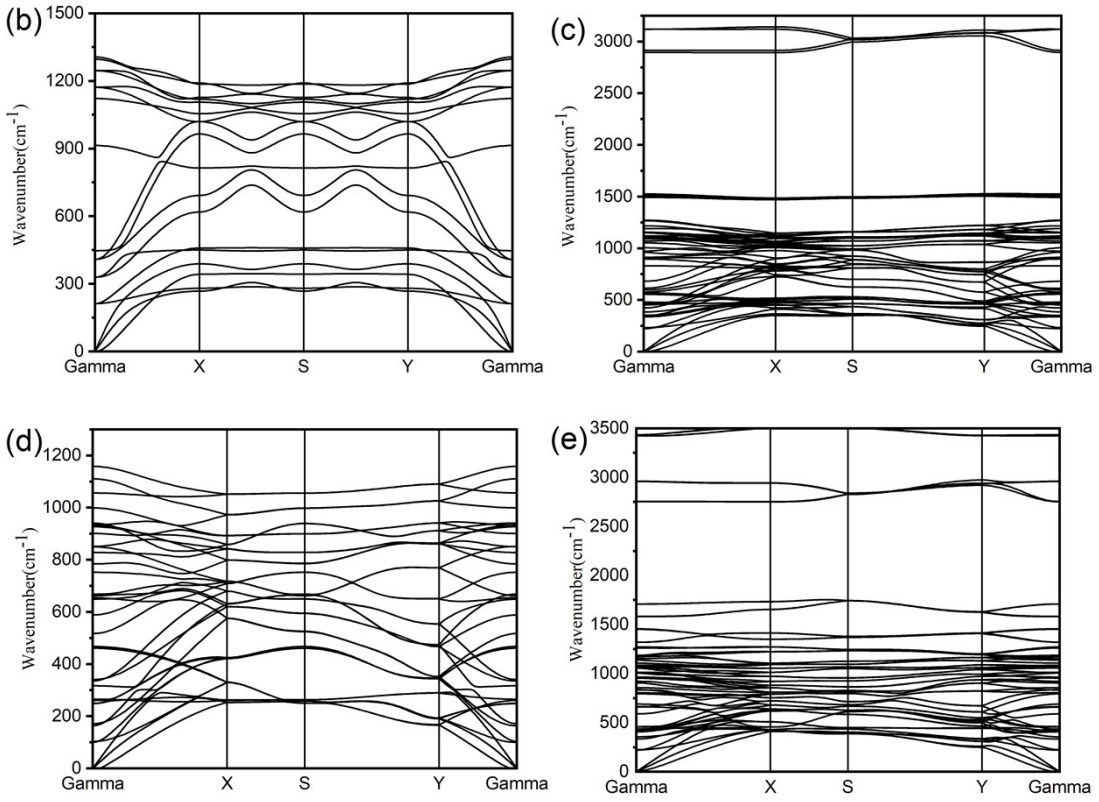


Fig. S2 phonon spectrums: (a) chair2-H (3◊3), (b) chair2-F (3◊3), (c) chair2-OH (3◊3), (d) chair2-Cl (5◊3), (e) chair2-NH_2 (3x3).

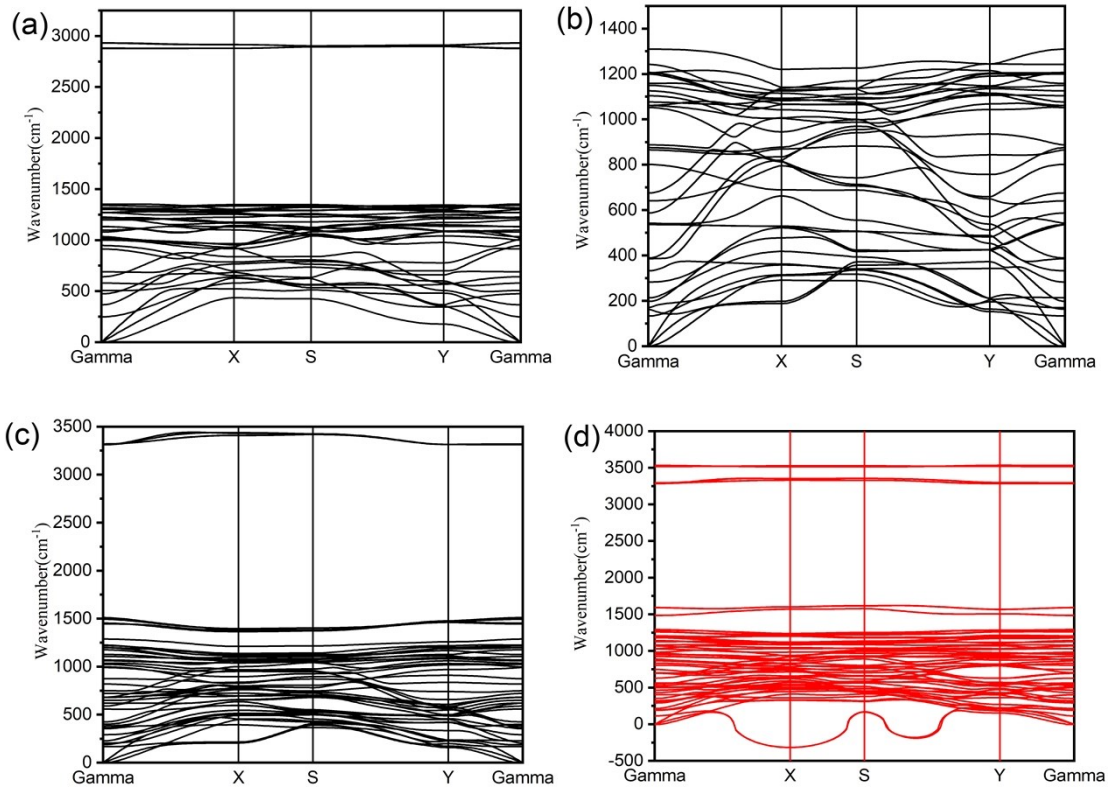


Fig. S3 phonon spectrums: (a) boat1-H (5◊3), (b) boat1-F (5◊3), (c) boat1-OH (5◊3), (d) boat1-NH_2 (5◊3).

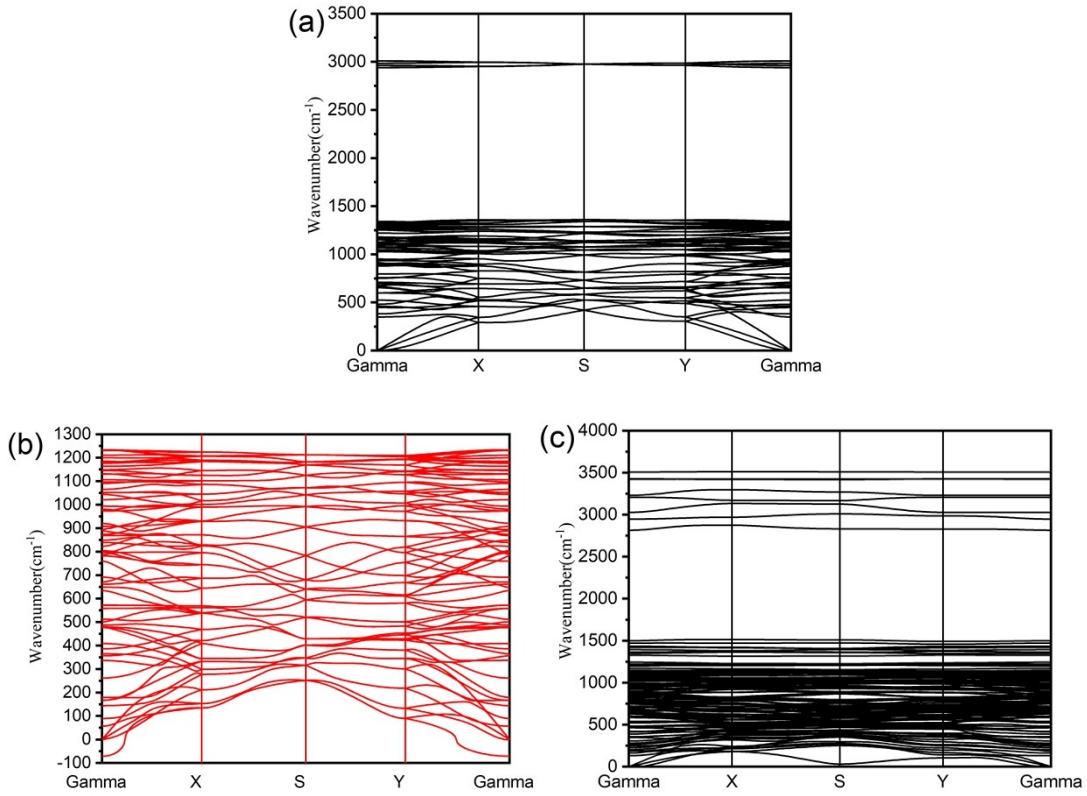


Fig. S4 phonon spectrums: (a) boat2-H (3◊3), (b) boat2-F (4◊4), (c) boat2-OH (4◊4).

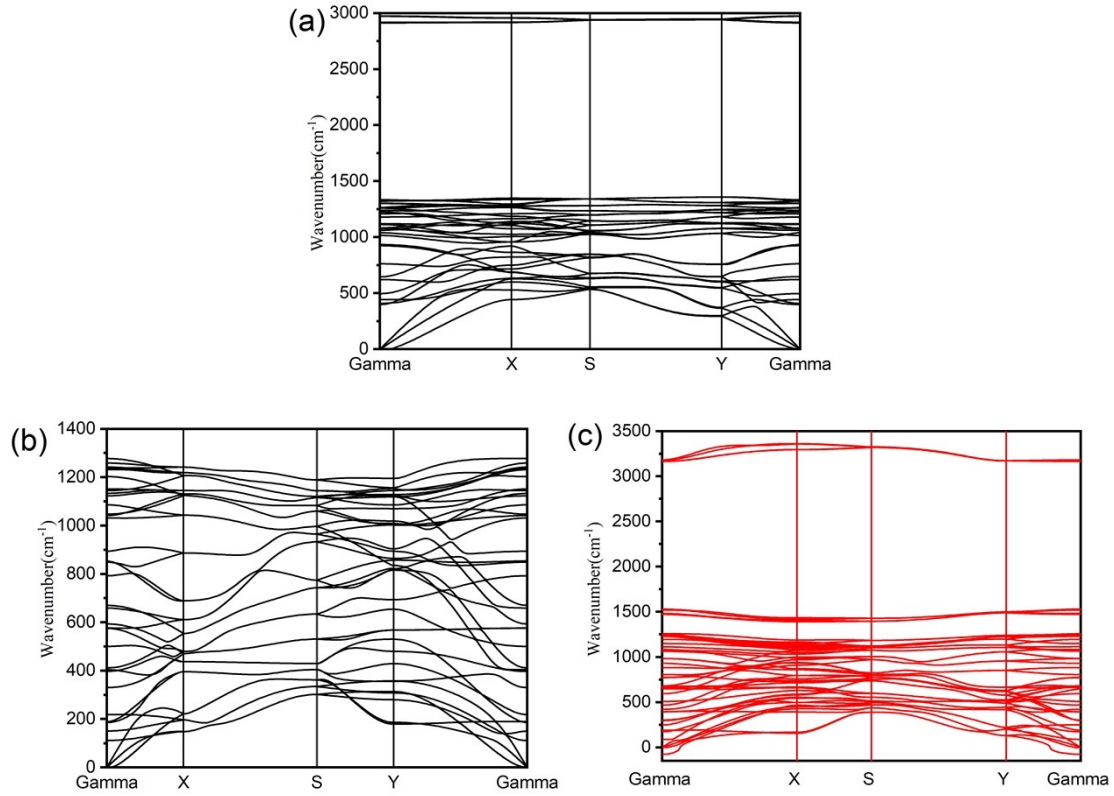


Fig. S5 phonon spectrums: (a) boat3-H (3◊5), (b) boat3-F (3◊5), (c) boat3-OH (6◊4).

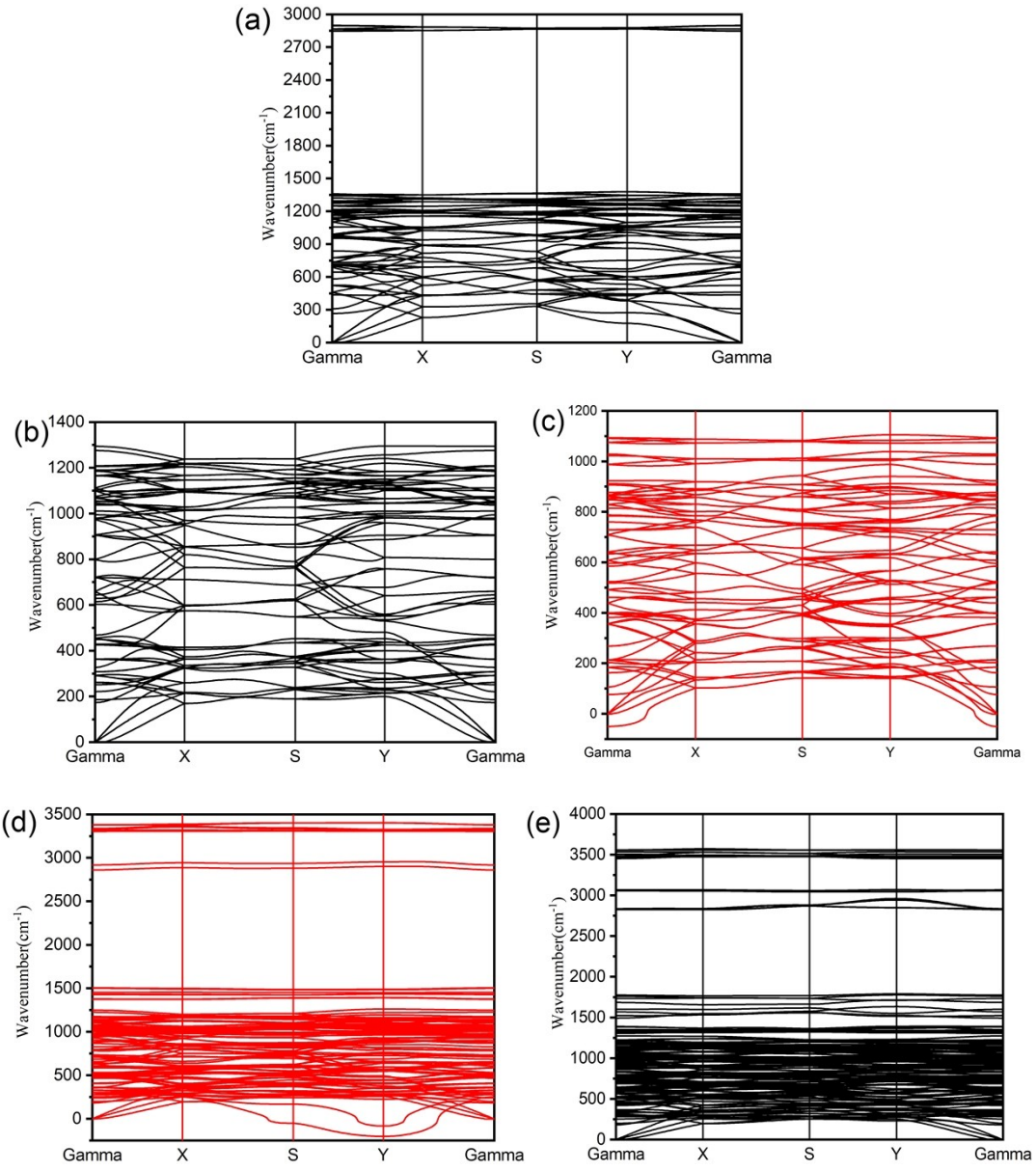


Fig. S6 phonon spectrums: (a) boat4-H (3◊3), (b) boat4-F (3◊3), (c) boat4-Cl (3◊4), (d) boat4-OH (3◊4), (e)boat4-NH_2 (3◊3).

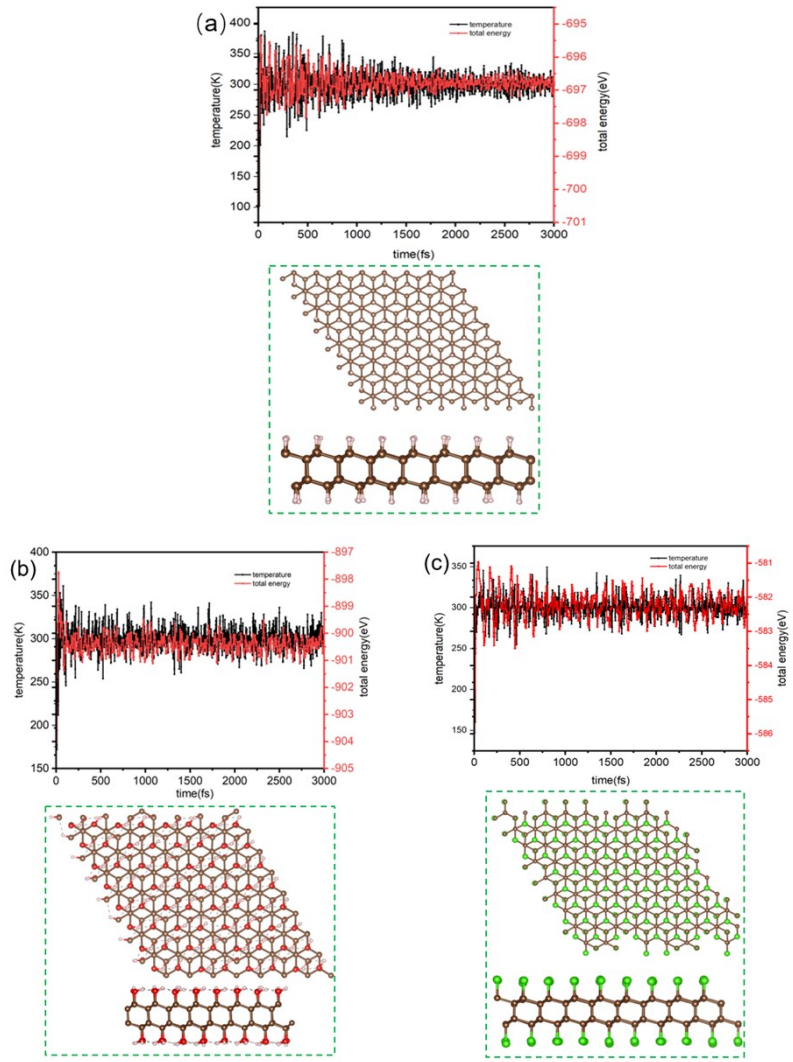
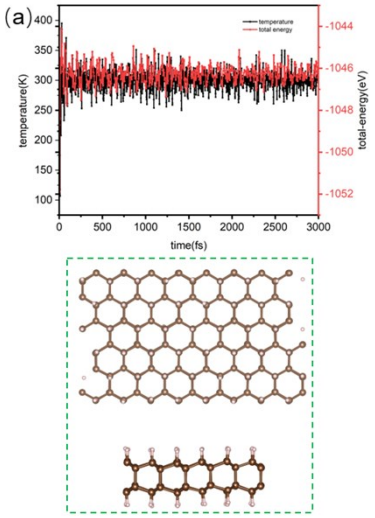


Fig. S7 phonon spectrums: (a) chair1-H, (b) chair1-OH, (c) chair1-Cl.



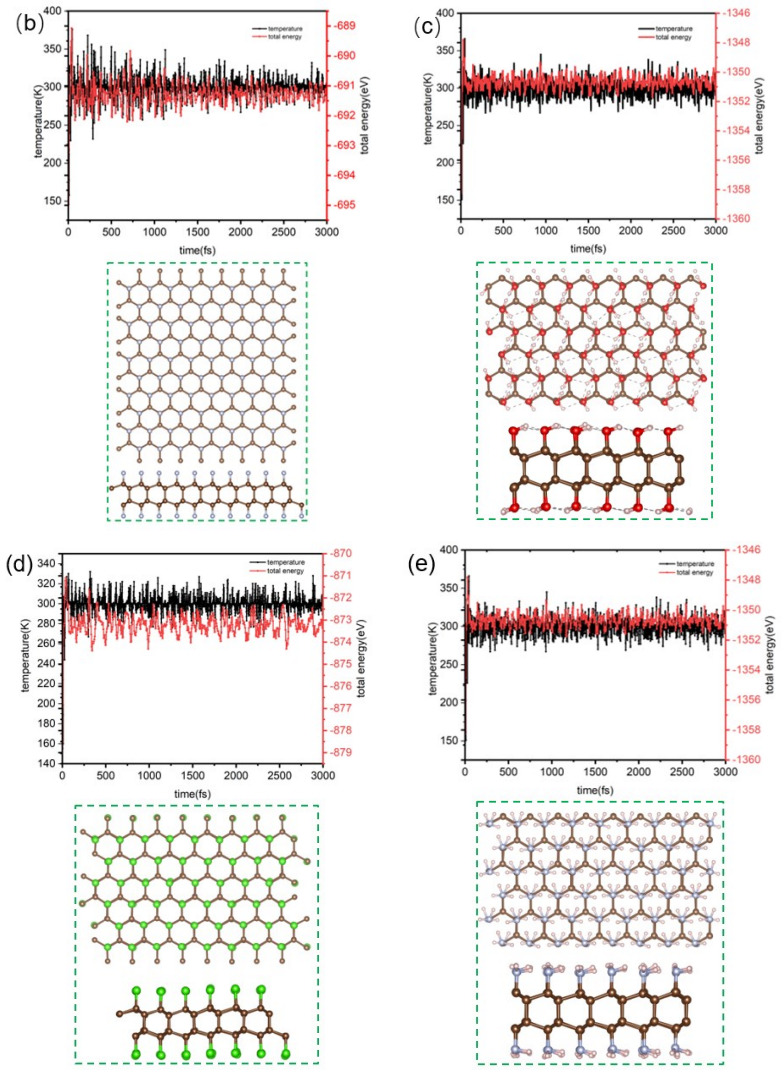
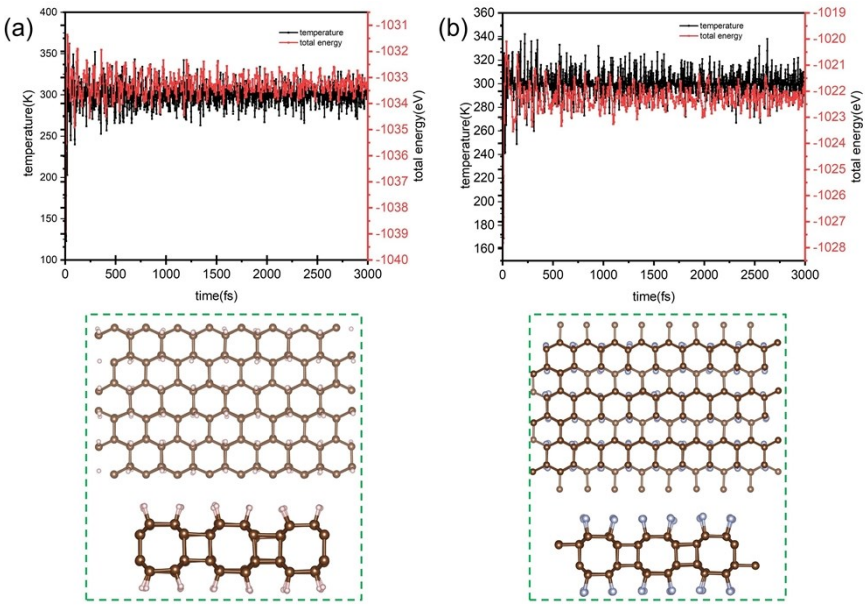


Fig. S8 The changes of energy and temperature with time and snapshots: (a) chair2-H, (b) chair2-F, (c) chair2-OH, (d) chair2-Cl, (e) chair2-NH_2.



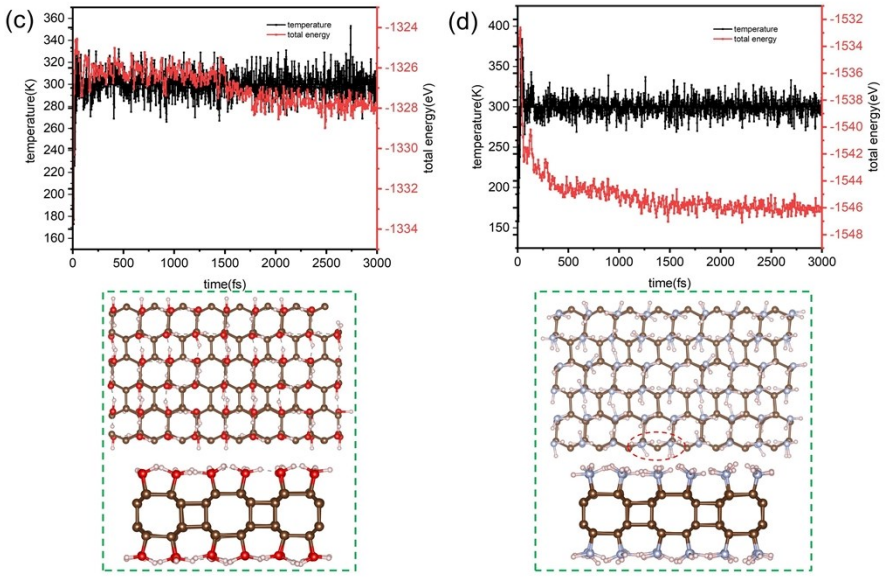
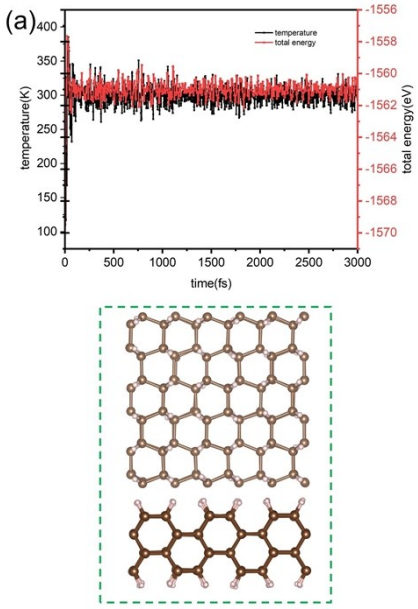


Fig. S9 The changes of energy and temperature with time and snapshots: (a) boat1-H, (b) boat1-F, (c) boat1OH, (d) boat1-NH_2.



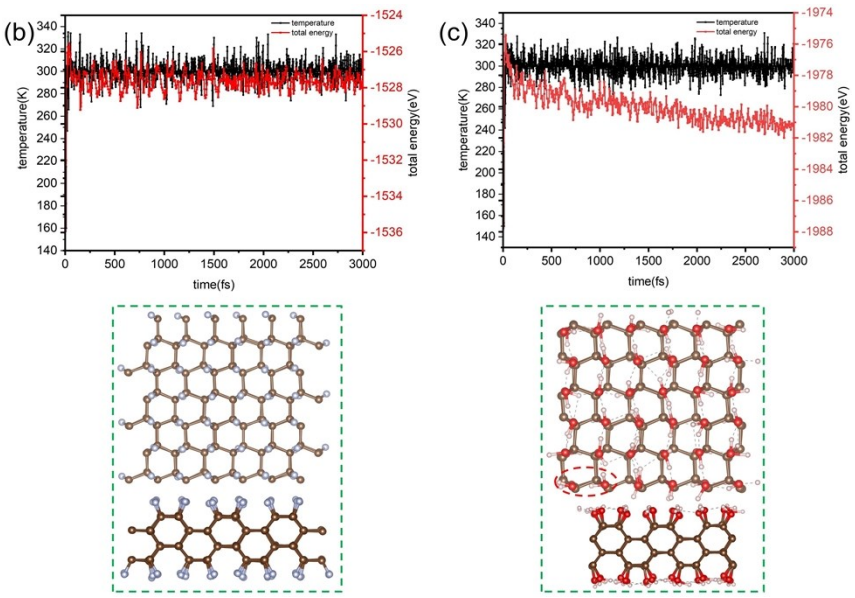


Fig. S10 The changes of energy and temperature with time and snapshots: (a) boat2-H, (b) boat2-F, (c) boat2-OH.

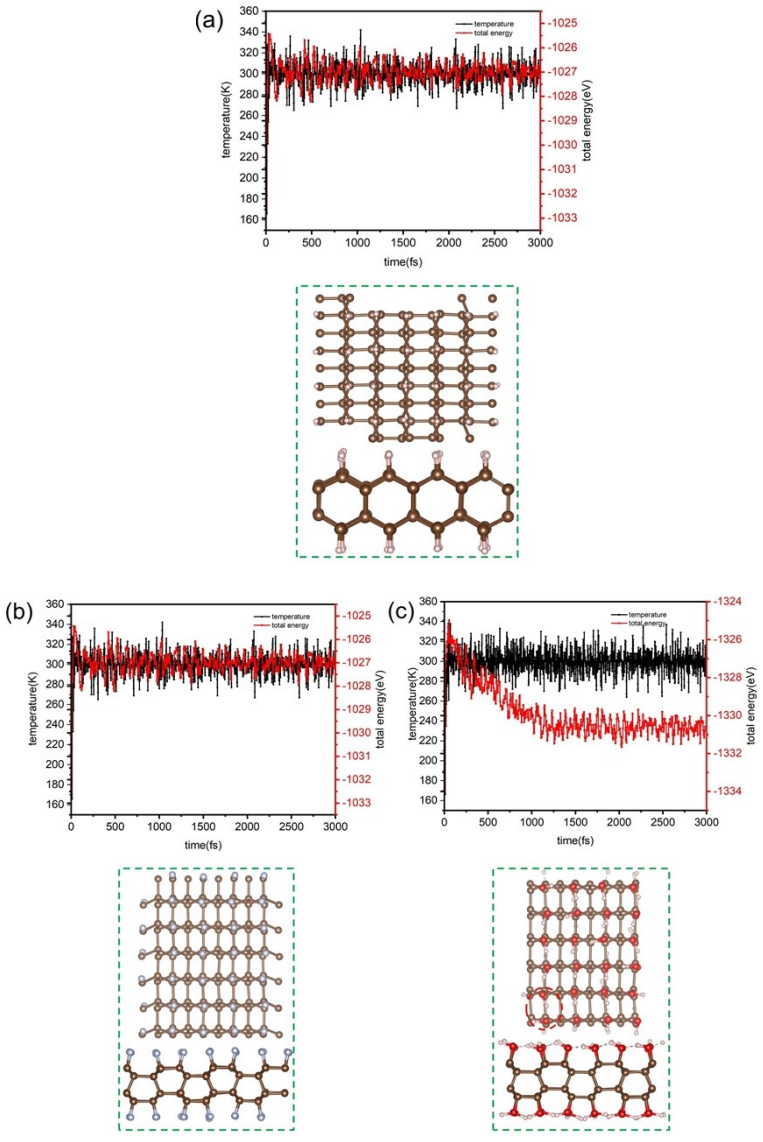
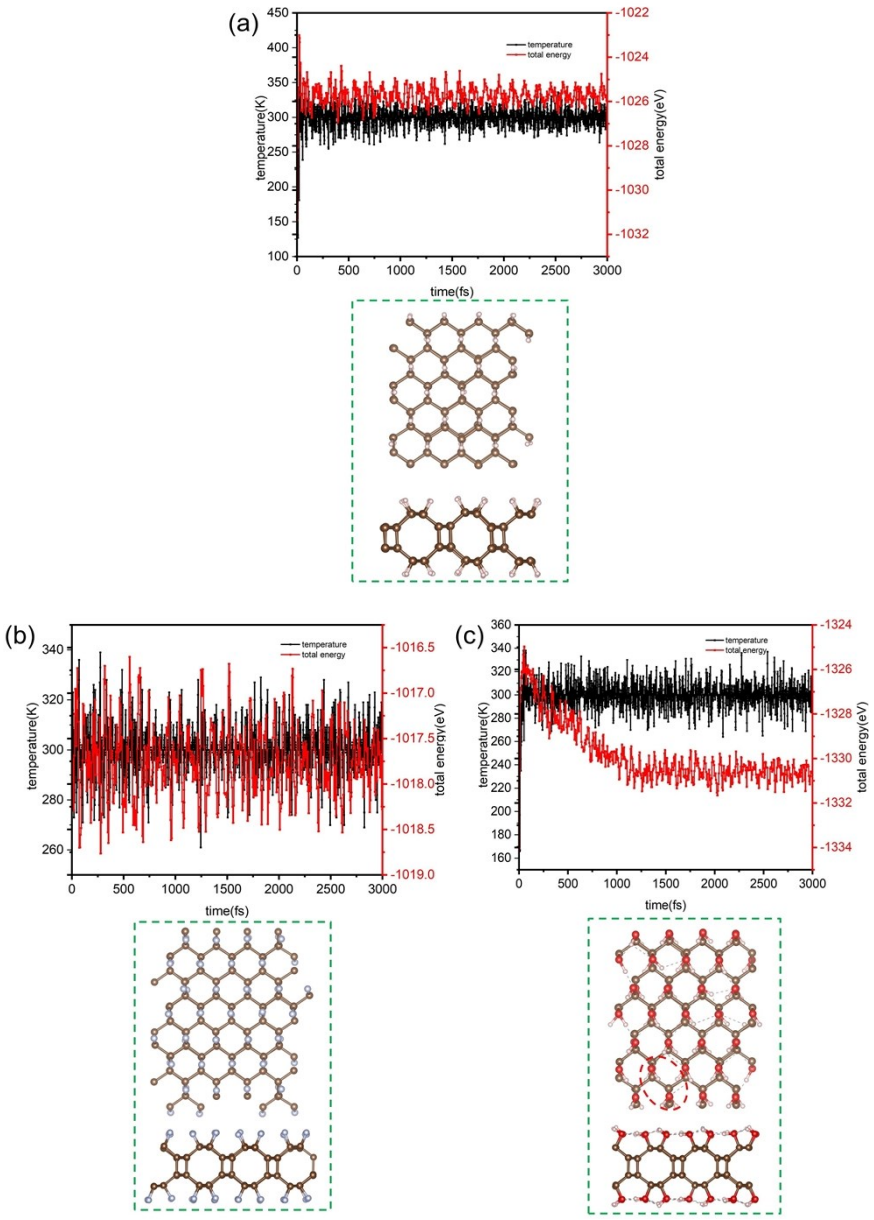


Fig. S12 The changes of energy and temperature with time and snapshots: (a) boat3-H, (b) boat3-F, (c) boat3-OH.



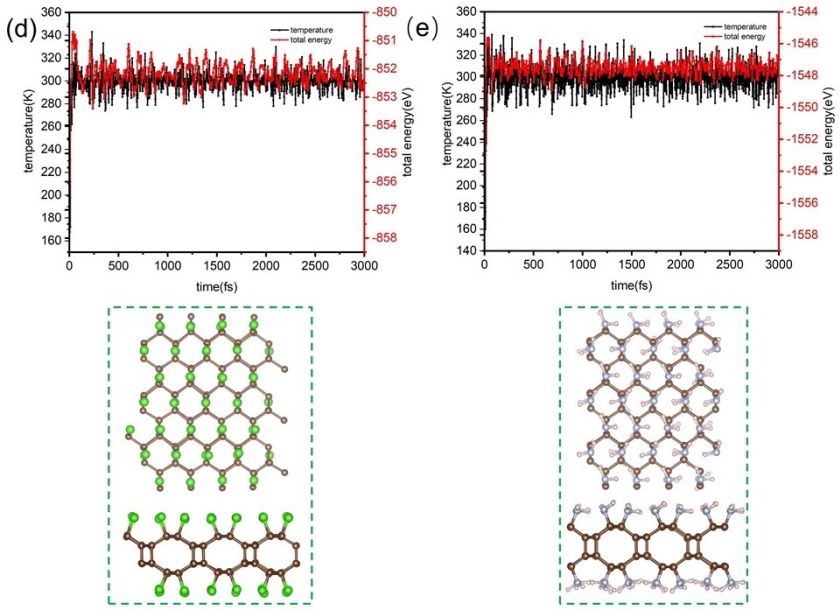


Fig. S13 The changes of energy and temperature with time and snapshots: (a) boat4-H, (b) boat4-F, (c) boat4-OH, (d) boat4-Cl, (e) boat4-NH_2.

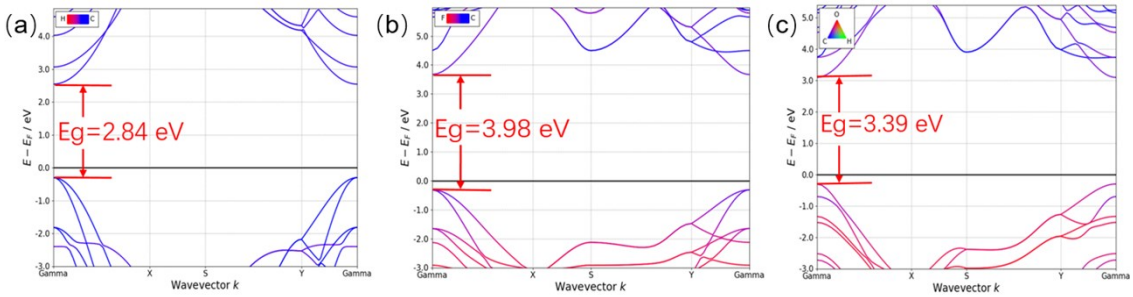


Fig. S14 The band structures: (a) chair2-H, (b) chair2-F, (c) chair2-OH.

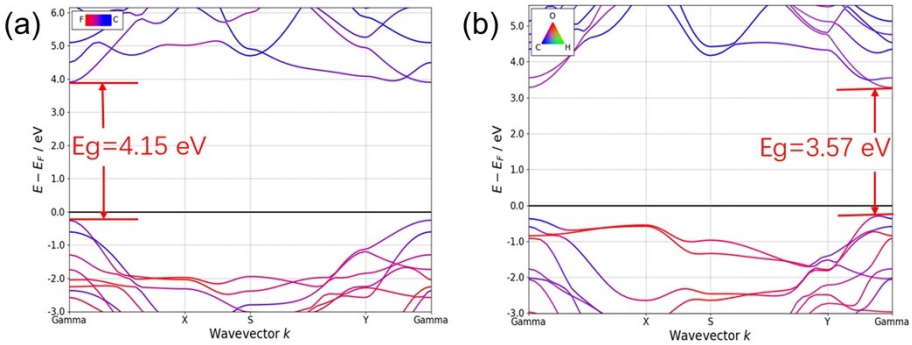


Fig. S15 The band structures: (a) boat1-F, (b) boat1-OH.

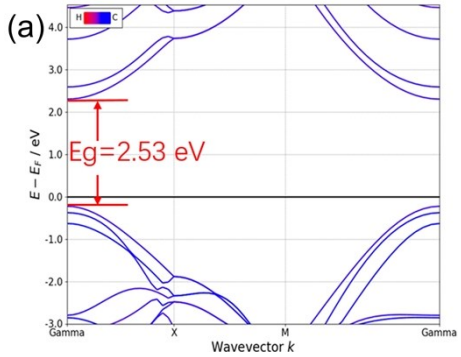


Fig S16. The band structures: (a) boat2-H.

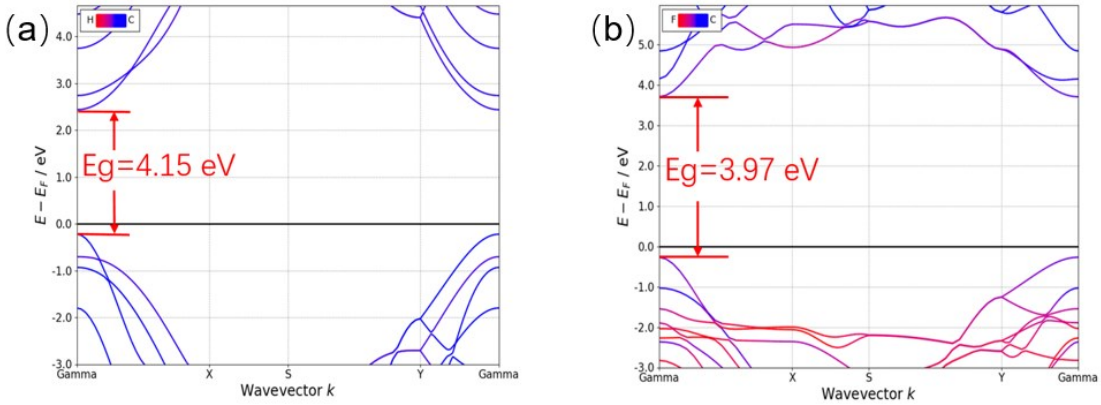


Fig S17. The band structures: (a) boat3-H, (b) boat3-F.

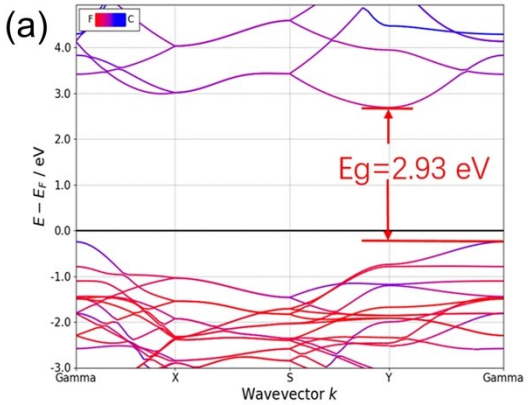


Fig. S18 The band structures: (a) boat4-F.

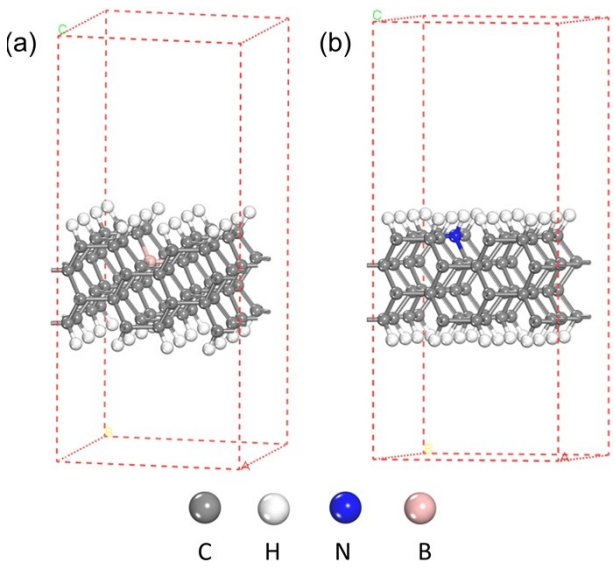


Fig. S19 Models of boat2-H: (a) B-doped, (b) N-doped.

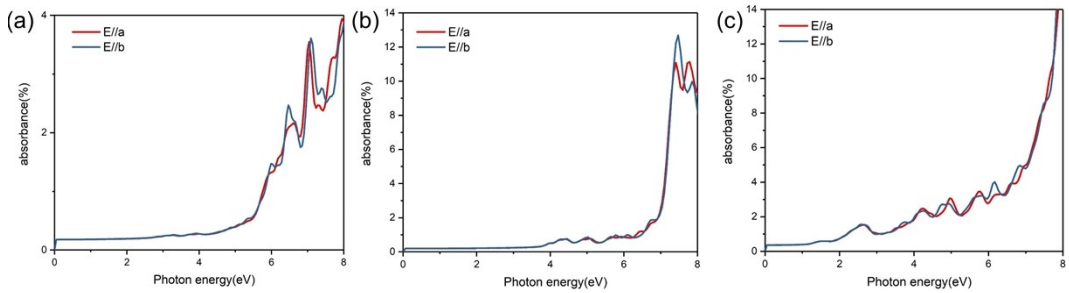


Fig. S20 The absorbance spectrum: (a) chair2-H, (b) chair2-F, (c) chair2-OH.

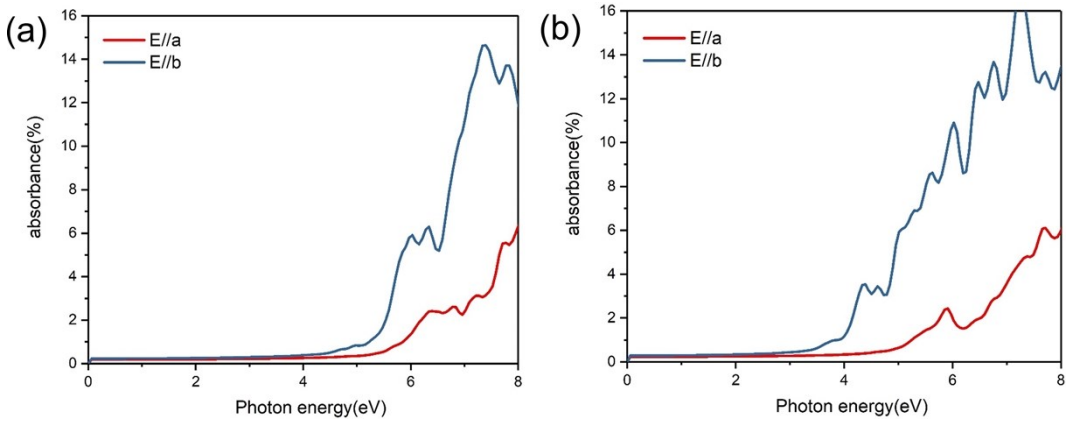


Fig. S21 The absorbance spectrum: (a) boat1-F, (b) boat1-OH.

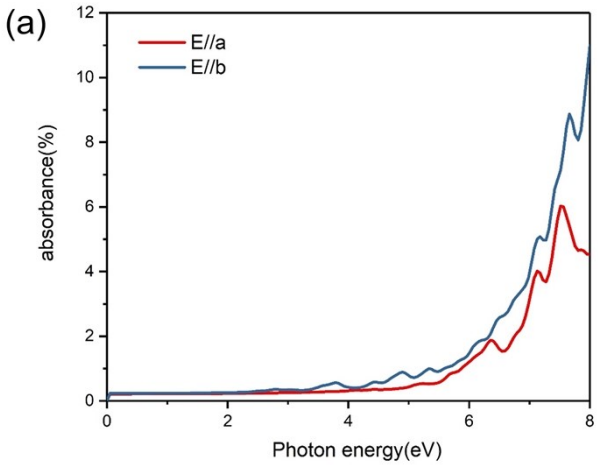


Fig. S22 The absorbance spectrum: (a) boat2-H.

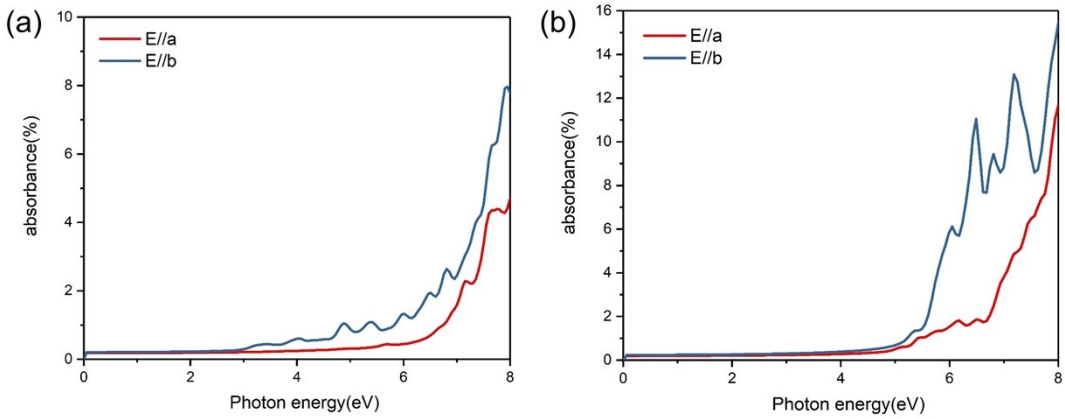


Fig. S23 The absorbance spectrum: (a) boat3-H, (b) boat3-F.

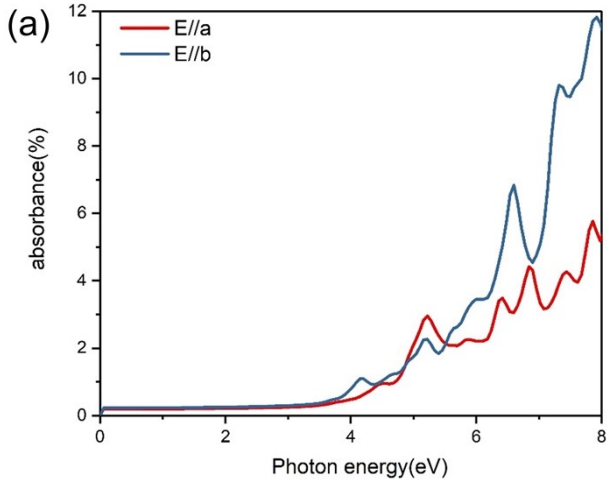


Fig. S24 The absorbance spectrum: (a) boat4-F.