Supporting Information For

Snatching the Ligand or Destroying the Structure: Disruption of WW Domain by Phosphorene

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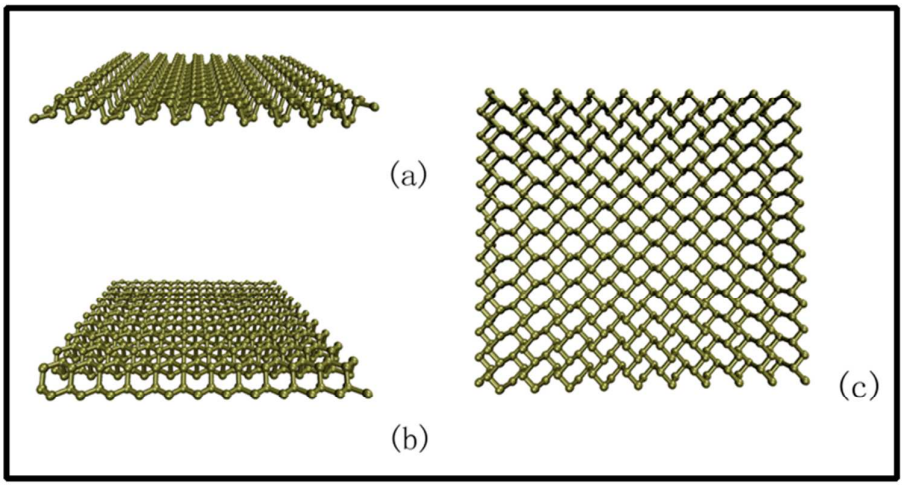

Figure S1: The configuration of phosphorene from different direction.

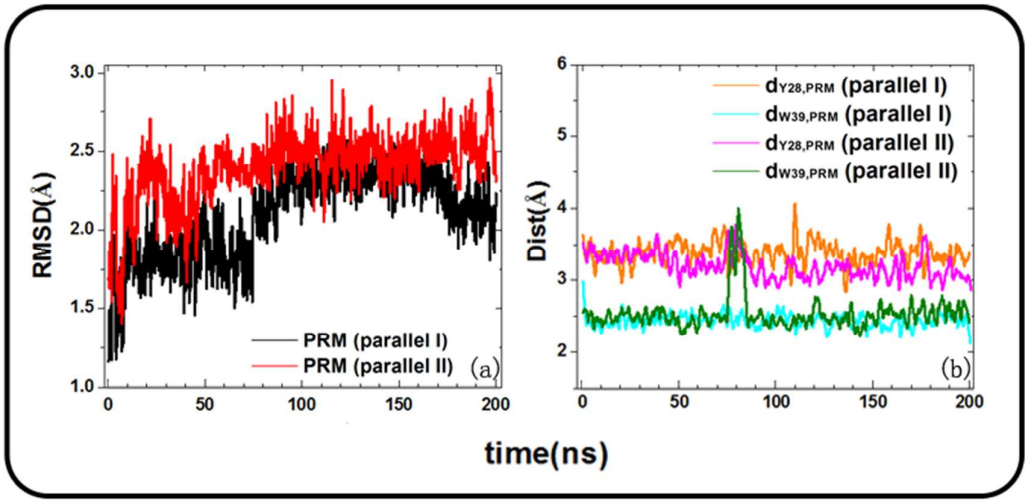

Figure S2: (a) The RMSD in the parallel I (black) and parallel II (red) model. (b) The distance between the PRM and two key residues, $d_{Y28,PRM}$ (orange) and $d_{W39,PRM}$ (cyan) in parallel I model , $d_{Y28,PRM}$ (olive) and $d_{W39,PRM}$ (purple) in parallel II model.

The RMSD and distance between the PRM and two key residues (Y28 and W39) in parallel I and parallel II model are computed. Fig. S1a shows that the structure of WW domain are steady with a low value in RMSD (> 2.5 Å). And the $d_{Y28,PRM}$ and $d_{W39,PRM}$ are steady too, in the Fig.S1 b. It illustrates WW domain kept a good binding state with PRM.

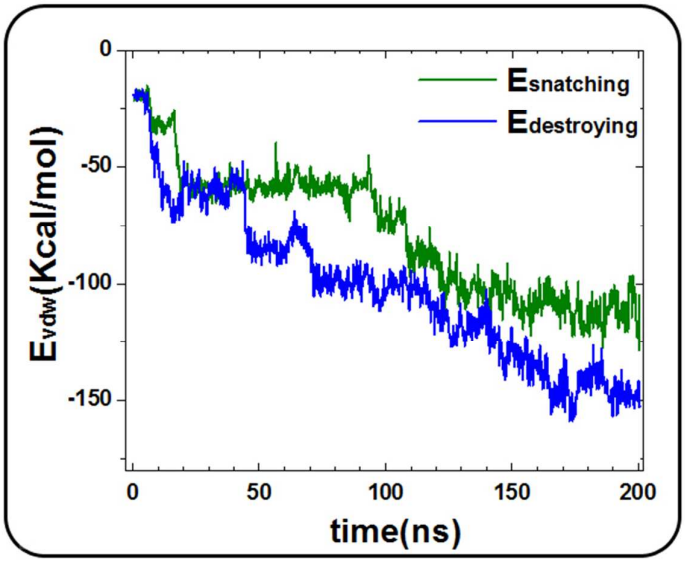

Figure S3: The van der Waals energy in the two disruption forms: snatching form $E_{snatching}$ (green line) and disruptive form $E_{destroying}$ (blue line)

The van der Walls energy E_{vdw} ($E_{PRM,WW} + E_{PRM,P} + E_{WW,P}$) in two disruption forms, denoted as $E_{snatching}$ and $E_{destroying}$.