

Supporting Information

Revealing the biotoxicity of phosphorene oxide nanosheets based on the villin headpiece

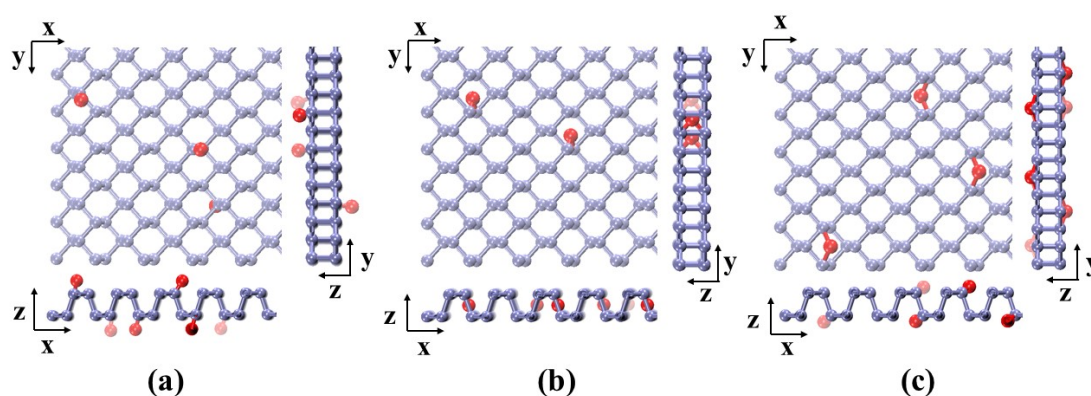


Figure S1. Oxidation mode of phosphorene nanosheet. (a) Dangling oxidation (Mode I). (b) Interstitial oxidation (Mode II). (c) Horizontal bridge oxidation (Mode III).

Table S1. Charge Distribution in PO nanosheets

Oxidation Mode	Phosphorus/e	Oxygen/e
Dangling oxidation	0.21	-0.21
Interstitial oxidation	0.08	-0.16
Horizontal bridge oxidation	0.09	-0.18

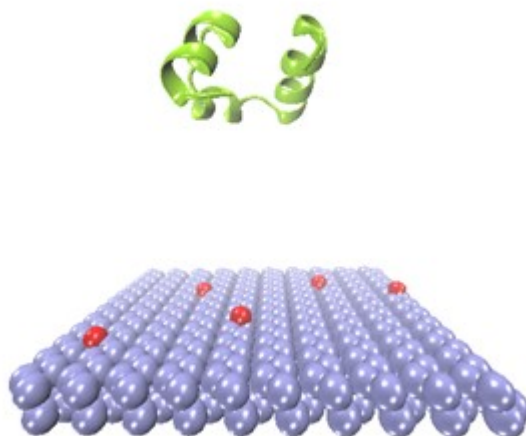


Figure S2. A complex composed of phosphorene oxide (Mode I) and HP35. The red, blue and yellow spheres represent oxygen atoms, phosphorus atoms and HP35, respectively.

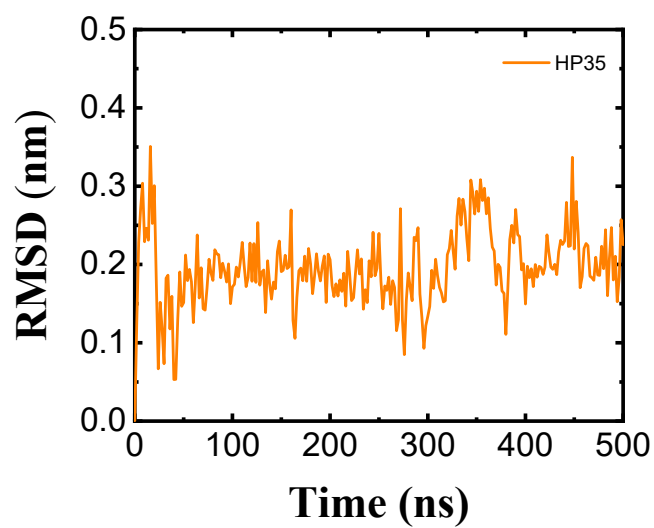


Figure S3. The root mean square deviation (RMSD) of protein HP35 in the absence of nanomaterials.

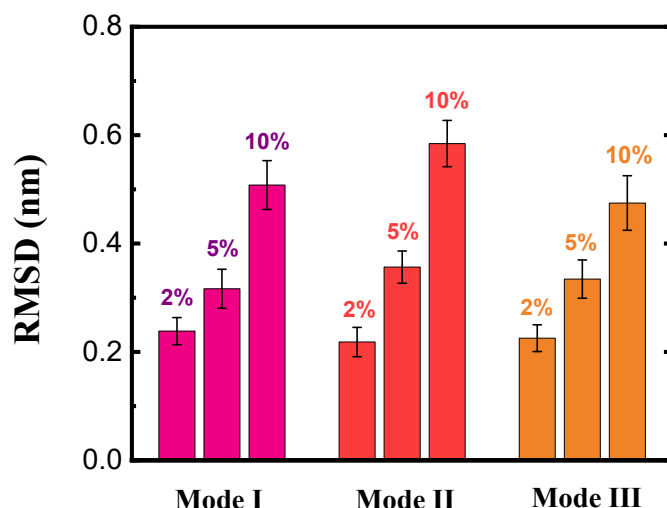


Figure S4. The mean RMSD of protein HP35 adsorbed on the surface of PO nanosheets in Modes I, II and III with oxidation concentrations of 2%, 5% and 10%.

As shown in Figure S4, the oxidation mode of PO has little effect on the RMSD of HP35 for a certain oxidation concentration of PO. The oxidation concentration of PO, however, has a significant effect on the RMSD of HP35. The greater the oxidation concentration of PO, the greater the RMSD of HP35 is, indicating that the disruption of PO to HP35 increases as the oxidation concentration increases. In the oxidation modes I, II and III of PO, the RMSD of HP35 varies with the oxidation concentration in the same trend.

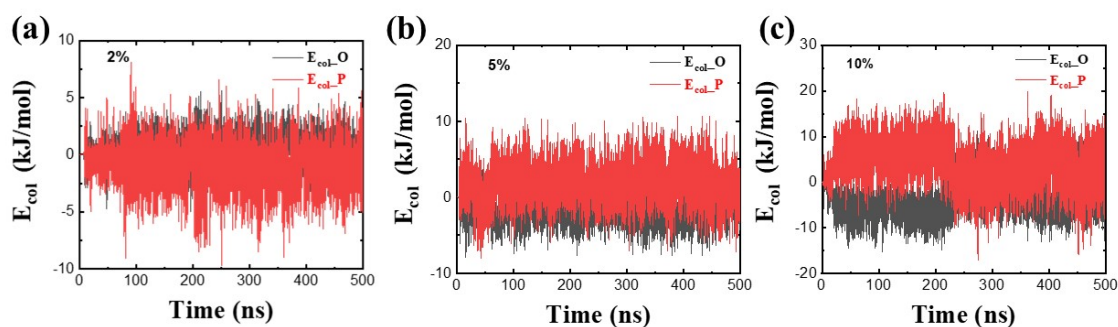


Figure S5. The Coulomb interaction energy between HP35 and oxygen atoms and phosphorus atoms of PO with Mode II and oxidation concentrations of (a) 2%, (b) 5% and (c) 10%.