

Supplementary Material

Remarkable Improvement in Phosgene Detection with Defect-Engineered Phosphorene Sensor: First- Principles Calculations

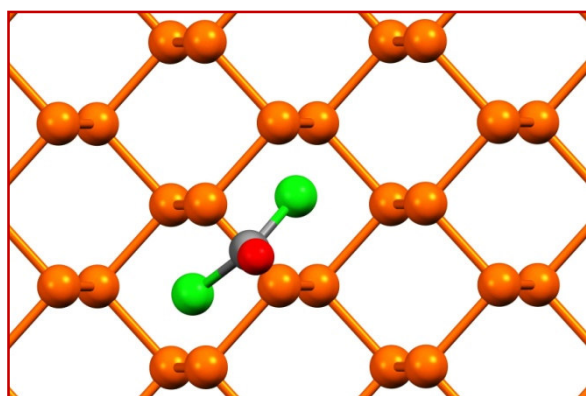
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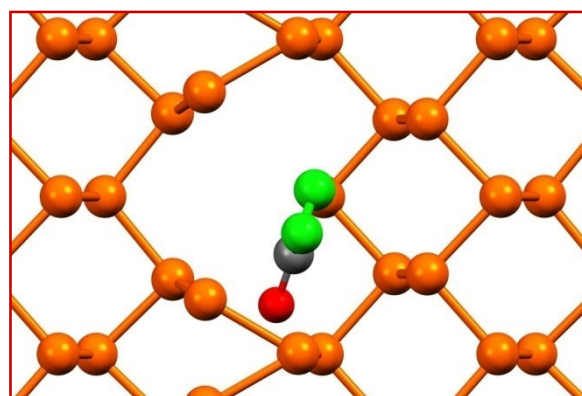
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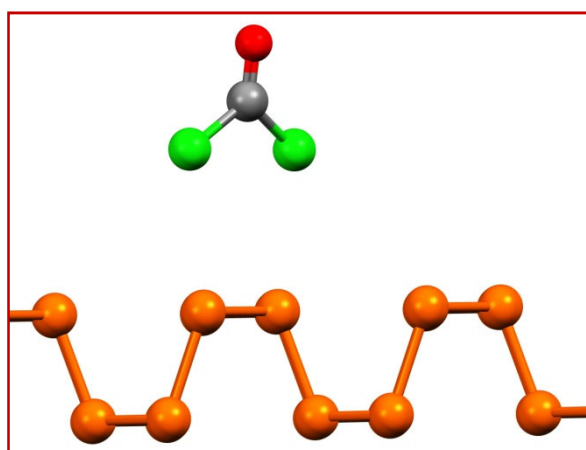
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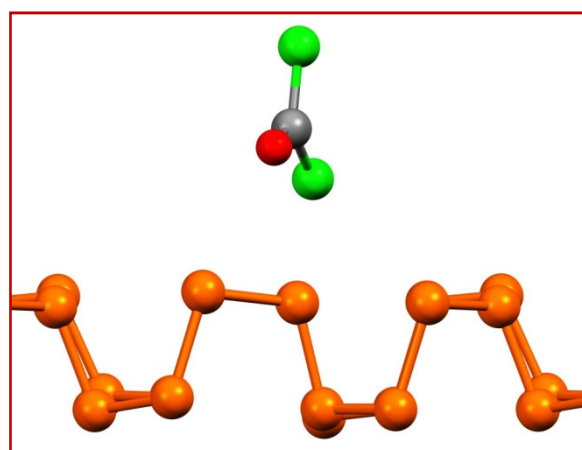
P1a (Top View)



P2a (Top View)

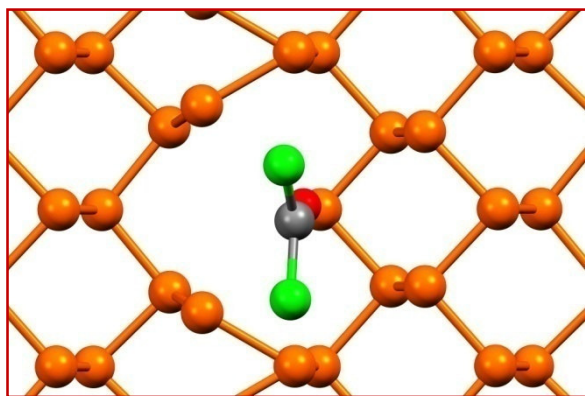


P1a (Side View)

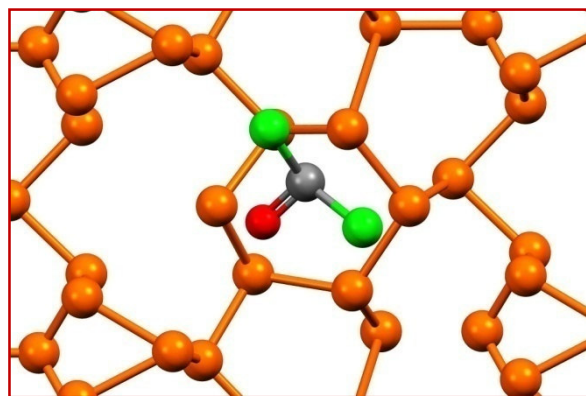


P2a (Side View)

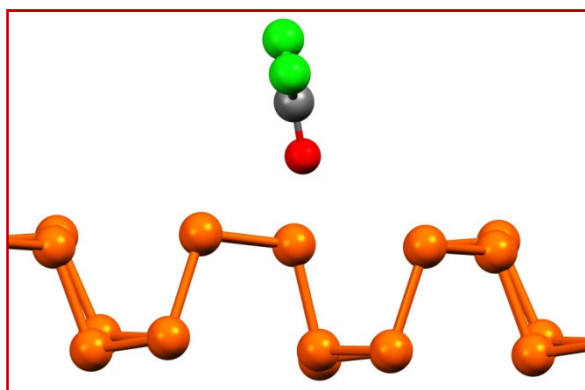
Figure S1. Alternative configurations for the phosgene stabilization on phosphorene sensors at the PBE/SVP level of theory.



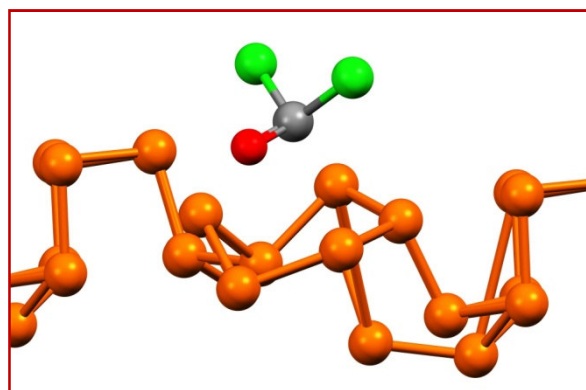
P2b (Top View)



P2c (Top View)



P2b (Side View)



P2c (Side View)

Figure S1. Contd.

Table S1. Calculated adsorption and binding energies (eV) for alternative adsorption structures of less thermodynamic favorability for the phosgene molecule on phosphorene-based sensors at the HSE06/TZVP level of theory.

Structure	ΔE_{ads} (eV)	ΔE_{b} (eV)
P1a	-0.04	0.05
P2a	-0.12	0.05
P2b	-0.12	0.05
P2c	1.24	3.85