

Supplementary Material

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

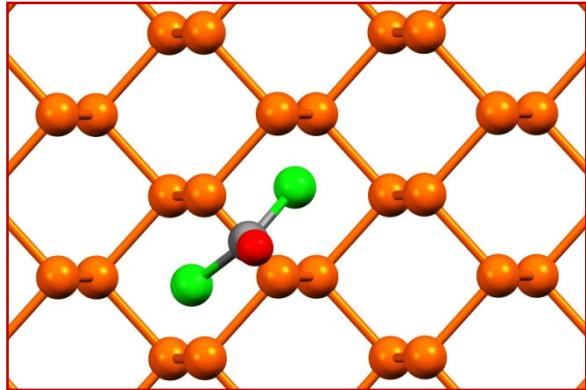
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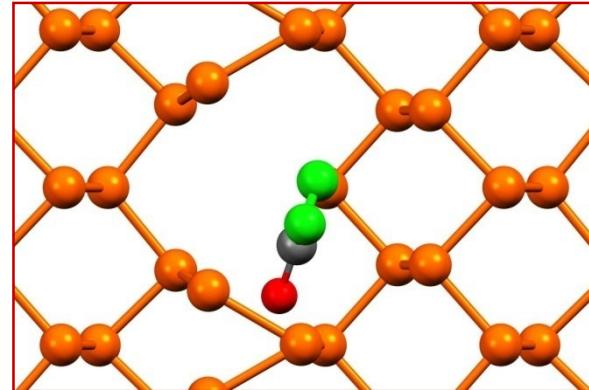
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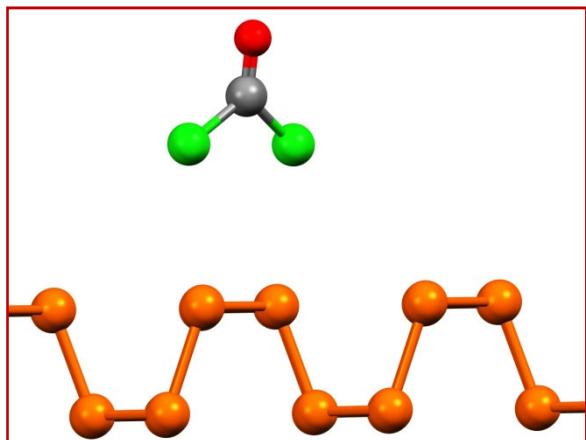
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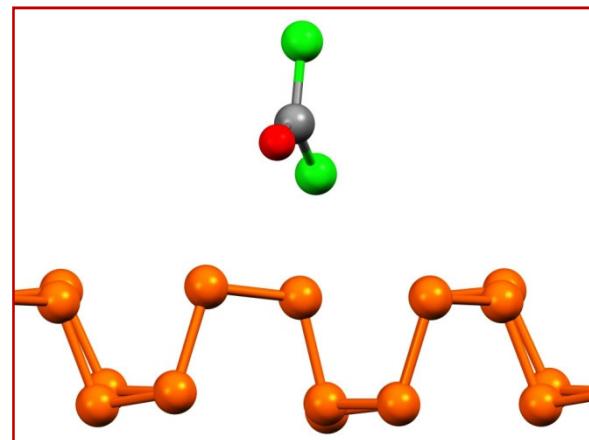
P1a (Top View)



P2a (Top View)

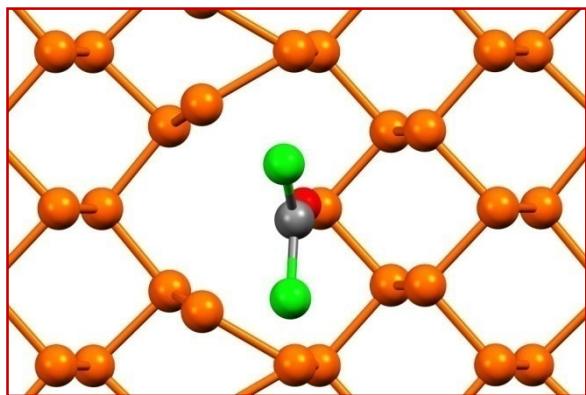


P1a (Side View)

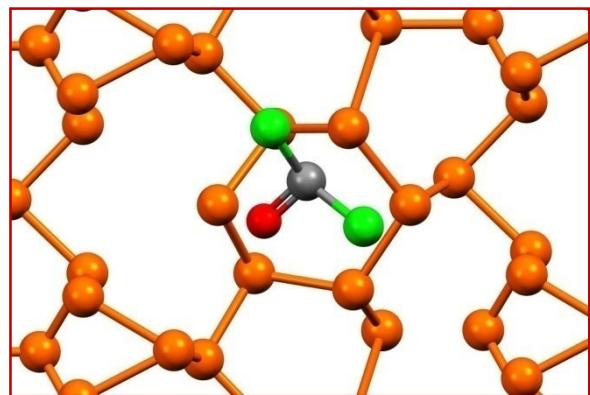


P2a (Side View)

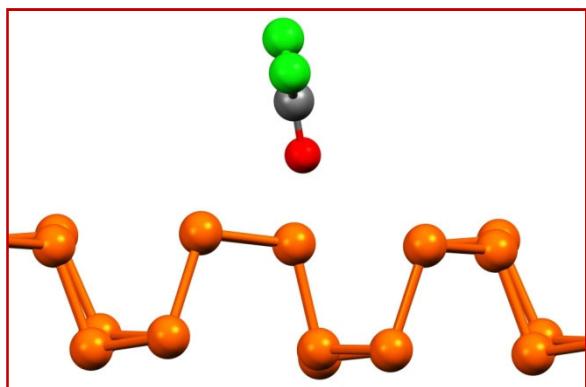
**Figure S1.** Alternative configurations for the phosgene stabilization on phosphorene sensors at the PBE/SVP level of theory.



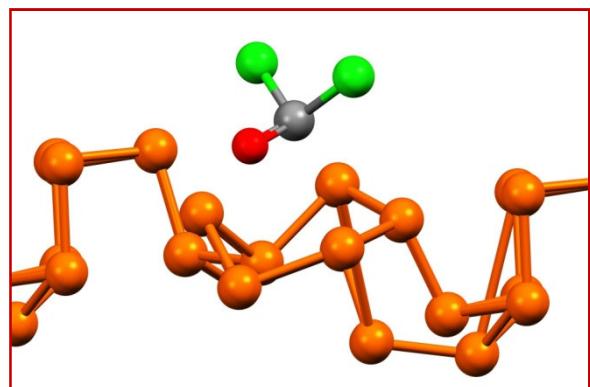
P2b (Top View)



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	$\Delta E_{\text{ads}}$ (eV)	$\Delta E_{\text{b}}$ (eV)
P1a	-0.04	0.05
P2a	-0.12	0.05
P2b	-0.12	0.05
P2c	1.24	3.85