2022
9(2), 132-137

Journal of
MATERIALS NANOSCIENCE

Sensing ability of Liquefied Petroleum Gas by Epsilon phosphorene nanosheets - a DFT investigation

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Supplementary information

Table S1. Comparison of sensing response of various phosphorene allotropes towards different target molecules.

Phosphorene Allotropes	Target Molecules	Adsorption energy range (eV)	Maximum Sensing Response (%)	References
Kagome phosphorene	Chloropicrin, Phosgene	-0.065 to -0.606	58.28	[1]
Black Phosphorene	DDT, heptachlor	-0.197 to -0.604	4.50	[2]
5-8 phosphorene	o-xylene, Styrene	-0.611 to -1.047	82.01	[3]
Black phosphorene	CO, CO_2, NO, NO_2, NH_3, H_2, O_2	-0.110 to -0.963	-	[4]
Green Phosphorene	1-bromo-2-butanone, Bromoacetone, Bromobenzyl cyanide	-0.170 to -0.273	22.53	[5]
Red tricycle Phosphorene	Sulfadiazine, Sulfamethoxazole	-2.874 to -4.641	22.73	[6]
Black Phosphorene	Thiophene	-0.24 to -0.50	-	[7]
Blue Phosphorene	CO, CO_2, NO, NO_2	-0.203 to -0.514	49.57	[8]
ε-PNS	**Propane, Butane**	**-0.376 to -0.766**	**34.96**	**Present Work**

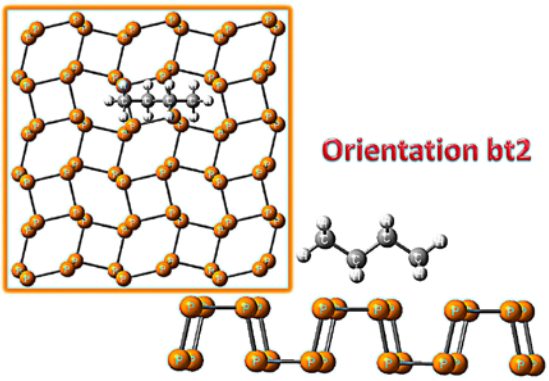

Figure S1 *Adsorption of butane on tetra site of* $\varepsilon - PNS -$ *orientation* $bt2$

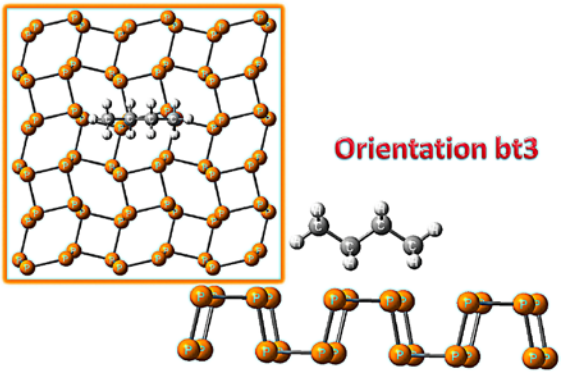

Figure S2 *Adsorption of butane on top site of* $\varepsilon - PNS -$ *orientation* $bt3$

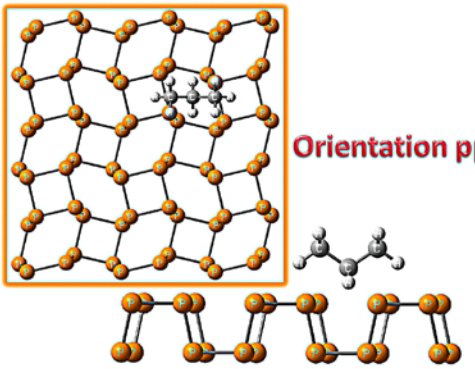

Figure S3 *Adsorption of propane on octa site of* $\varepsilon - PNS -$ *orientation* $pp1$

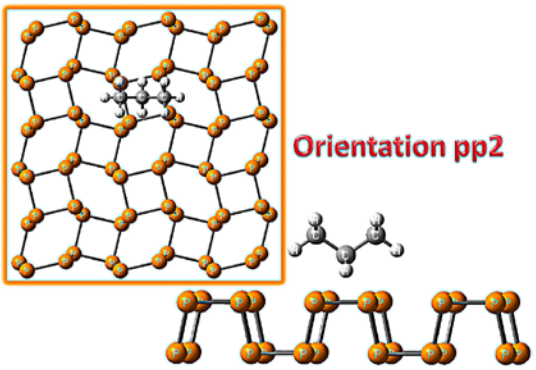

Figure S4 *Adsorption of propane on tetra site of* $\varepsilon - PNS -$ *orientation* $pp2$

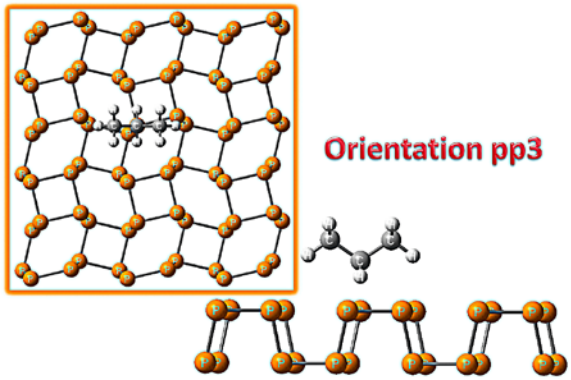

Figure S5 *Adsorption of propane on top site of ε − PNS − orientation pp3*

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