Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# The Potential Application of Black and Blue Phosphorene as Cathode Materials in Rechargeable Aluminum Batteries: a First-principles study

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**Table S1** Calculated open circuit voltage (OCV) of black and blue phosphorene with different $AlCl_4^-$ concentration ($(AlCl_4)_xP_n$; $x = 1, 2, 4$, and 8; $n = 16\ or\ 18$ for black or blue phosphorene, respectively).

| ***x*** | ***1*** | ***2*** | 4 | ***8*** |
|---|---|---|---|---|
| ***Black Phosphorene*** | 2.44 | 2.59 | 2.59 | 4.1 |
| ***Blue Phosphorene*** | 4.05 | 2.88 | 2.58 | 3.86 |

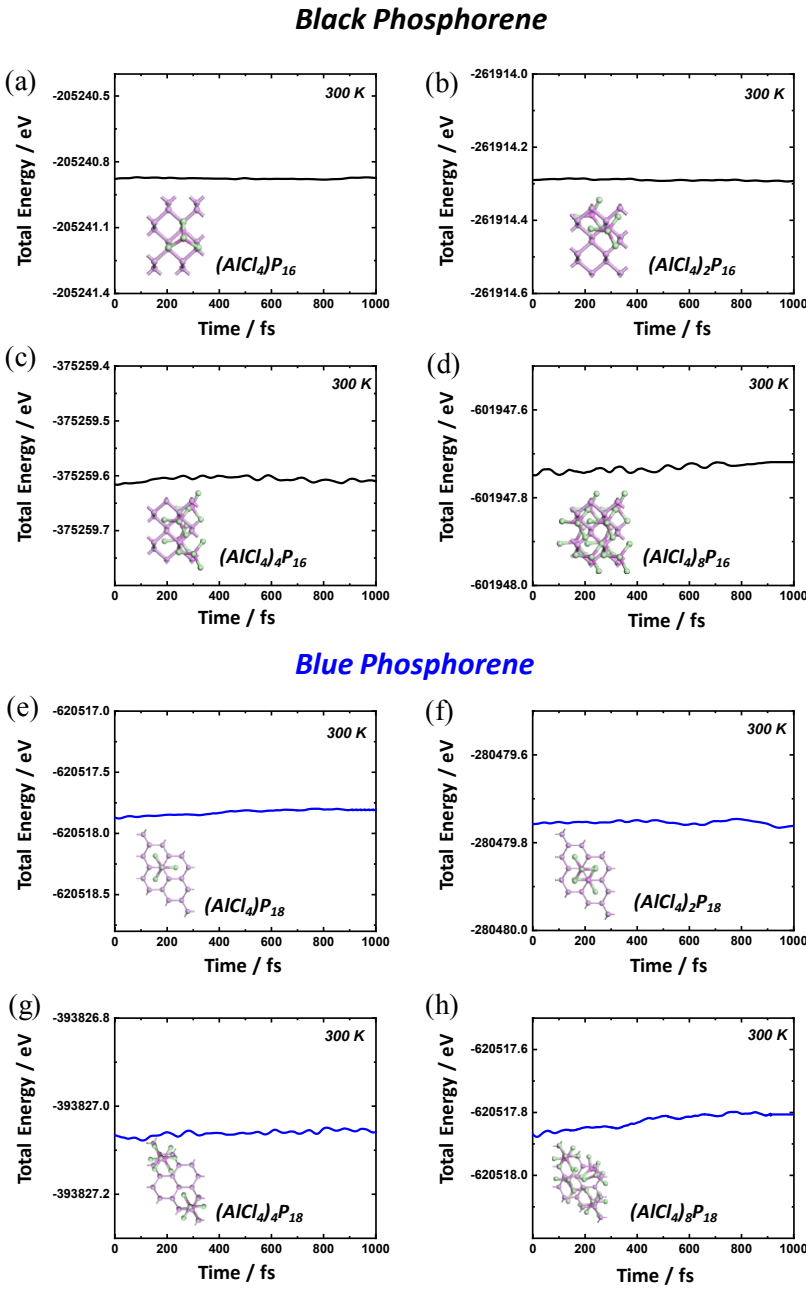


**Fig. S1** AIMD simulation analysis of black (a-d) and blue phosphorene (e-h) with multiple $AlCl_4^-$ adsorptions.