**Supplementary Information**

**DFT insights into the detection of NH3, AsH3, PH3, CO2, and CH4 gases with pristine and monovacancy phosphorene sheets**

**Figure S1:** The interaction energies of NH3, AsH3, PH3, CO2, and CH4 gas molecules on pristine phosphorene (P) (blue color) and mono vacancy phosphorene (MVP) (orange color) sheets.

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| **(A) P-NH3** | **(B) MVP-NH3** |
| **Figure S2:** Projected DOS of (A) P-NH3 and (B) MVP-NH3 adsystem. | |
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| **(A) P-AsH3** | **(B) MVP-AsH3** |
| **Figure S3:** Projected DOS of (A) P-AsH3 and (B) MVP-AsH3 adsystem. | |