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Supporting Information for

DFT coupled with NEGF Study of Ultra-sensitive HCN and HNC Gases detection and Distinct *I-V* Response based on Phosphorene

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1. Supporting Information for the selectivity of sensor device towards HCN, HNC, H_2O and O_2 gas molecules

The O_2 and H_2O gases are present rich at the ambient condition. In order to ascertain the selectivity of the phosphorene nanosensors toward HCN and HNC molecules, the I-V curves of H_2O and O_2 gas molecules have also been calculated for comparison. As shown in Fig. S1 and S2, the magnitude of transverse current varies widely when different gas molecules are put into the phosphorene. It is distinct that after the applied voltage is larger than threshold voltage, the value of current is obviously different when HCN and HNC adsorbed on the phosphorene, which is much larger than that of the H_2O and O_2 cases, so it is easy to distinguish HCN and HNC molecules from H_2O and O_2 molecules. For the armchair direction, the ranks of current values under 2.4 V for all devices are $I_{HCN} \approx I_{HNC} > I_{O_2} > I_{pure} > I_{H_2O}$. While for the zigzag direction, the ranks of current values under 2.4V are $I_{HNC} > I_{HCN} > I_{H_2O} > I_{O_2} > I_{pure}$. Therefore, it is easy to distinguish the HCN and HNC molecules conditions. Besides, we find that the discrimination ability for different species changes with bias voltages, thus, it is necessary to set an appropriate bias voltage to better sequence gas molecules in a real experiment.

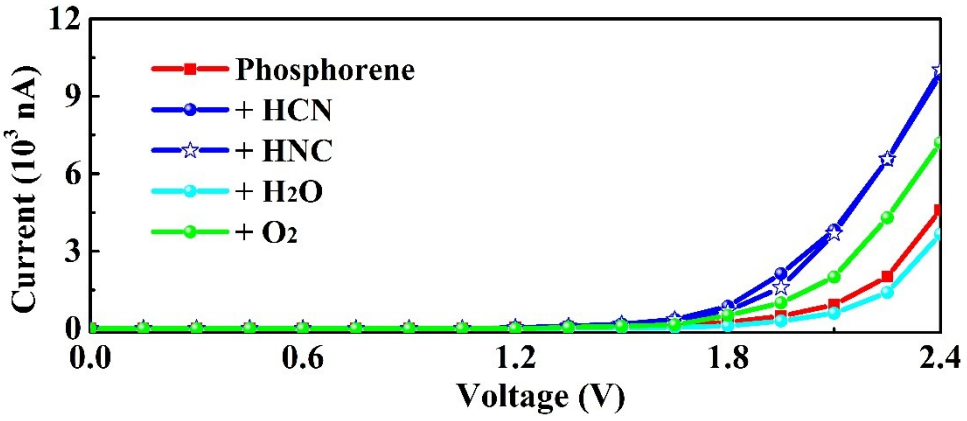

Fig. S1. The I-V curves of pristine phosphorene and with HCN, HNC, H_2O and O_2 molecule adsorption along the armchair direction.

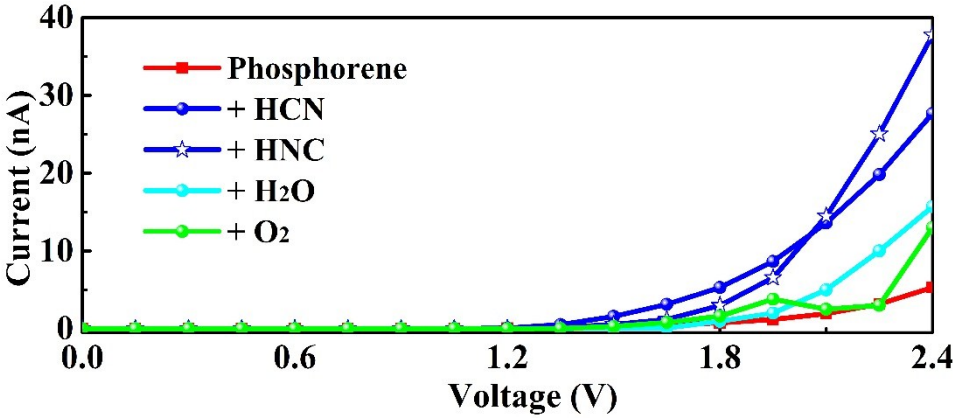

Fig. S2. The I-V curves of pristine phosphorene and with HCN, HNC, H_2O and O_2 molecule adsorption along the zigzag direction.