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Gas Sensors Based on Nanostructured Materials

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Abstract:

The concern with air quality and safety urges the design and development of new gas sensors. Low dimensional structures pose as promising new sensing materials due to their compatibility with portable devices, low power consumption, and superior sensitivity and selectivity. In this scenario, graphyne presents comparable electronic mobility and mechanical properties to graphene, with the advantage of naturally allowing single-atom dispersion into acetylenic pores. Therefore, we investigate the detection ability of transition metal (TM: Fe and Ni) doped graphyne (Gy) toward toxic gas molecules. As a result, we notice different binding energies and sensitivity among the gases, thus NiGyNR and FeGyNR present high selectivity to distinguish the target molecules. Finally, our findings suggest that TM functionalization of graphynes is a promising strategy for engineering the sensitivity of gas nanosensors.

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