Machine Learning-Enabled Smart Gas Sensing Platform for Identification of Industrious Gases

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Abstract

Both ammonia and phosphine are widely used in industrial processes, and yet they are noxious and exhibit detrimental effects on human health.[1] A variety of gas sensors have been developed to detect and monitor them in an industrial environment.[2,3] Despite the remarkable progress on sensors development, there are still some limitations, for instance, the requirement of high operating temperatures, and that most sensors are solely dedicated to individual gas monitoring.[4] Here, we demonstrate an ultrasensitive, highly discriminative platform for the detection and identification of ammonia and phosphine at room temperature using graphene nanosensor. Graphene is exfoliated and successfully functionalized by copper phthalocyanine derivate. In combination with highly efficient machine learning techniques, the developed graphene nanosensor demonstrates an excellent gas identification performance even at ultralow concentrations, 100 ppb NH_3 (accuracy-100.0%, sensitivity-100.0%, specificity-100.0%), 100 ppb PH_3 (accuracy-77.8%, sensitivity-75.0%, and specificity-78.6%). Molecular dynamics simulation results reveal that the copper phthalocyanine derivate molecules attached on the graphene surface facilitate the adsorption of ammonia molecules owing to hydrogen bonding interactions. The developed smart gas sensing platform paves a path to design a highly selective, highly sensitive, miniaturized, low-power consumption, non-dedicated, smart gas sensing system towards a wide spectrum of gases.

References

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[4]. Panes-Ruiz LA, et al. ACS Sens 3, 79-86 (2018).

Figures

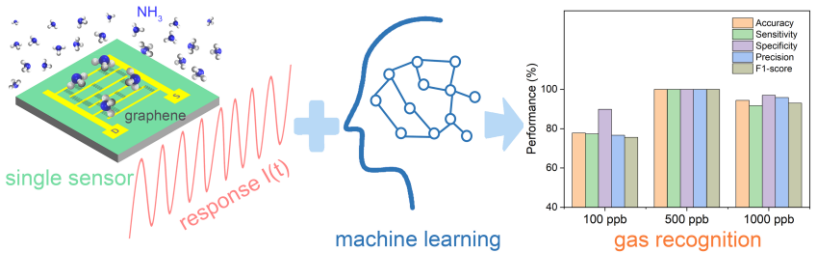

Figure 1: Schematic illustrations of the smart graphene nanosensor platform.