NH_3 and PH_3 Identification Using Graphene based Gas Sensor

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Abstract
Both NH_3 and PH_3 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 the NH_3/PH_3 gas in an industrial environment. [2-4] Despite the remarkable progress of sensors development, there are still some limitations, for instance, the requirement of high working temperature, and the dedication to solely individual gas monitoring. [5] Here we develop an ultrasensitive, highly discriminative platform for the detection and identification of NH_3 and PH_3 at room temperature using a graphene nanosensor. Graphene is exfoliated and successfully functionalized by a copper phthalocyanine derivate (CuPc). In combination with efficient machine learning techniques, the developed graphene nanosensor demonstrates an excellent gas identification performance even at ultralow concentration, 100 ppb NH_3 (accuracy-100%, sensitivity-100%, specificity-100%) and 100 ppb PH_3 (accuracy-77.8%, sensitivity-75%, and specificity-78.6%), as shown in Figure 1. Molecular dynamics simulation results reveal that the attachment of CuPc on the graphene surface facilitates the adsorption of NH_3 owing to hydrogen bonding interactions. This smart-sensor prototype paves a path to design highly discriminative, ultrasensitive, miniaturized, non-dedicated gas sensors towards a wide spectrum of industrious gases.

References

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Figures

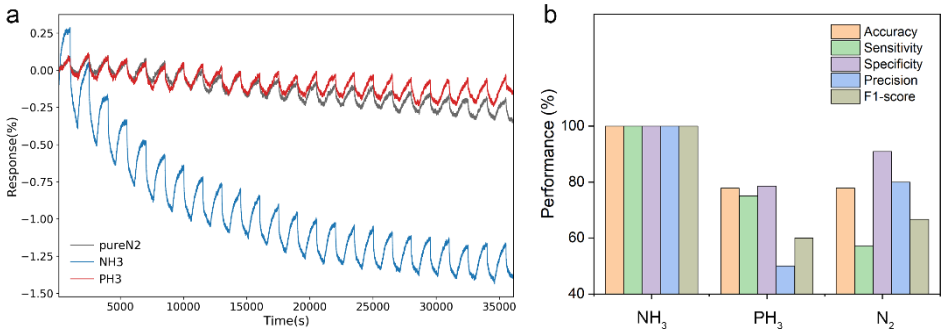

Figure 1. (a) Sensor response towards 100 ppb analyte gas (NH_3, PH_3 and N_2). (b) Sensor performance metrics towards analyte gas at their 100 ppb concentration using hold-out cross-validation method.