Design of Highly Responsive Room-Temperature Gas Sensors through Organic Layer-Graphene Interfaces

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Highly sensitive and selective gas-sensing materials are critical for applications such as environmental monitoring and medical diagnostics. To overcome the limitations of current metal oxide semiconductor technologies [1] - which, despite their widespread commercial use, require high operating temperatures for optimal performance - a rational nanoscale design approach is urgently needed to develop next-generation sensing devices. [2]

In this presentation, we explore the interface between p-type doped graphene and a nickel phthalocyanine (NiPc) molecular layer (Figure 1) through a combined computational and experimental approach, highlighting its potential for gas sensing applications. [3,4]

Using density functional theory calculations, we first examined the response of the graphene-NiPc interface to adsorbed gas molecules. NH_3 and NO_2 were chosen as representative test molecules, acting as electron donors and acceptors, respectively. Our analysis revealed that the Ni d_{z^2} orbital plays a crucial role in facilitating charge transfer and modulating graphene's charge carrier density.

As a proof of concept, we prepared a graphene-NiPc chemiresistor device and tested its performance at room temperature. The device exhibited excellent sensitivity and selectivity, rapid recovery times, and an impressively low detection limit, highlighting its potential for practical gas sensing applications.

References

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Figures

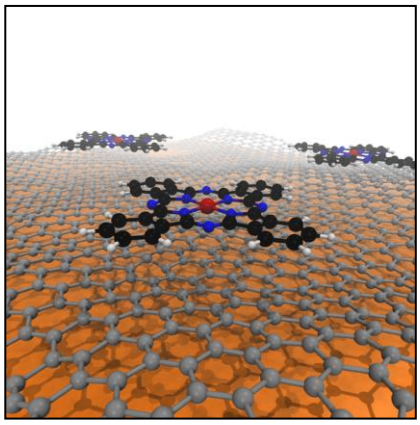

Figure 1: Ball-and-stick model illustrating the interface between a graphene monolayer and nickel phthalocyanine (NiPc) molecules.