Abstract

Volatile organic compounds (VOCs) are a diverse array of organic chemicals associated with industrial processes, vehicle emissions, and biological activities. The detection and monitoring of their evolution are crucial for applications in environmental monitoring, industrial safety, and healthcare diagnostics. Their presence in food products determines the quality and freshness of food. Thus, the detection and separation of VOCs emitted by food are intricately related to the assessment of spoilage through continuous monitoring of their concentrations.

The unique electrical properties and atomically thin layers of two-dimensional (2D) materials make them outstanding candidates in this field. Because of their chemical diversity, structural adaptability, quantum confinement, high surface-to-volume ratios, and ease of surface modification, large-surface-area 2D materials have drawn significant attention.

This thesis investigates these possibilities by computing the sensing capabilities of diverse 2D materials using first-principles density functional theory (DFT) and non-equilibrium Green's function (NEGF) theory for standard food products. The goal is to classify these 2D materials into different sensing mechanisms, namely chemiresistive sensors, work-function-based sensors, and optical sensors.

We find that while pristine graphene performs poorly as both a chemiresistive and work-function-based sensor, r-GO in either mode is able to differentiate between four out of six VOCs. It turns out that GO, on the other hand, performs at par with r-GO as a work-function-based sensor but is not useful as a chemiresistive one. The analysis based on electronic structures, structural parameters, and adsorption characteristics traces such behavior back to the hybridization of molecular orbitals driven by the adsorption geometry.

Subsequently, the sensing and electronic properties of silicene and F-silicene are explored. This study reveals how functionalization drastically changes the electronic properties of the material, which impacts the charge transfer and transport properties. Next, we investigate the sensing properties of MXene and MXene/TMDC heterostructures. We show that sensitivity increases upon the formation of heterostructures. By forming heterostructures, a large charge transfer occurs across the interface compared to the case of bare MXene. This, coupled with significant changes in the work function, leads to much better sensitivities in heterostructure-based sensors.

Finally, we investigate the role of MXenes in sensing the food quality of papaya fruit. MXene, a new class of 2D material, has drawn considerable attention due to its unique structural properties. Different functional groups on the MXene surface behave differently in sensing food quality by altering the electronic and optical properties of the sensor.

In summary, this thesis expands our understanding of how 2D materials and their functionalization impact sensing properties toward volatile organic compounds emitted from standard food products through changes in electronic structure, charge transfer, and optical properties.