

## **Atomistic simulation of a non-covalent functionalized graphene-based material for body odor volatiles detection**

Detecting the body odor volatiles (BOVs) represents a crucial step in comprehending its implications for human social interactions and healthcare. This work explores a novel mucin-based receptor functionalized graphene-based sensor material for BOVs detection through atomistic simulations. The density functional theory (DFT) investigation involves calculating the binding features of analyte-substrate interactions, including binding energy and charge transfer. These electronic properties characterize the sensing mechanisms and yield synergistically sensor signal response in the end, which could be estimated by the work function change before and after BOVs adsorption. This research enhances the fundamental understanding of the analyte-receptor interactions and potentially facilitates the selection and optimization of the receptors in pursuit of high responsiveness and excellent discrimination capabilities.

**Keywords:** DFT; functionalized graphene; BOV; adsorption; work function;