

Atomistic simulation of olfaction-receptor functionalized graphene for body odor volatiles detection

Body odor volatiles (BOVs) are the VOCs compounds emitted from human body, such as breath, urine, and skin. They are pivotal biomarkers for diagnosing several threatening human diseases such as Parkinson's and Alzheimer's. Therefore, a robust material for detecting the BOVs is desired, which plays a crucial step in the early and non-invasive medical diagnosis and even prevention of threatening human diseases. Inspired by the mammalian olfaction system, 18 olfactory receptors were designed and synthesized at HUJI university to detect a broad spectrum of skin odor molecules.

This work explores the biomimetic odorant-receptor functionalized graphene sensor materials for BOVs adsorption through atomistic simulation. To initialize the workflow, 102 skin odor molecules with defined physicochemical descriptors were screened. Molecular docking was used to generate initial odorant-receptor configurations, and then the density functional theory (DFT) was conducted to investigate the odorant-receptor interaction on graphene, where binding features including descriptors related to structure, energy, charge, and surface potential were obtained.

First, the binding features for these physisorption systems were shown to be uncorrelated. Then, correlating the binding features with the structural and chemical properties of the odorants revealed the potential for strong discrimination by the receptor molecules. For example, structurally and/or chemically similar molecules could exhibit different binding features.

Furthermore, machine learning methods were utilized to discover the binding features space and obtain sensitivity and selectivity information of receptors towards different body odor molecules. This research enhances the fundamental understanding of the analyte-receptor interaction mechanism and potentially facilitates the estimation of the discrimination capabilities of the olfaction receptors towards different BOVs.