

# Machine Learning-enabled 2D Nanomaterials-based Electronic Olfaction Sensors and Their Applications

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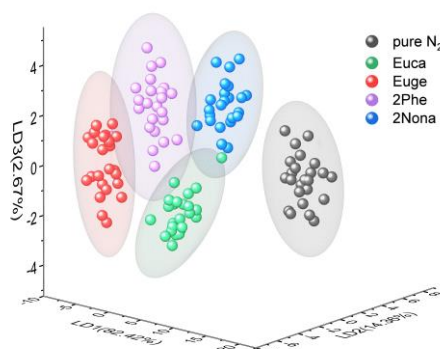
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Olfaction is an evolutionary old sensory system, which provides sophisticated access to information about our surroundings. Inspired by the biological example, gas sensors in combination with efficient machine learning algorithms aim to achieve similar performance and thus to digitize the sense of smell. Despite the significant progress of e-noses, their compactness still remains challenging due to the complex layout design of sensor arrays with a multitude of receptor types or sensor materials, and the high working temperature. In this talk, we present the development of machine learning-enabled graphene-based single-channel electronic olfaction (e-olfaction) sensors and propose a methodology to evaluate their olfactory performance. We selected four VOC-based odors, namely eucalyptol, 2-nonanone, eugenol, and 2-phenylethanol, which are widely used in human olfactory performance assessment. We achieved a low odor detection limit of 4.4 ppm (for 2Phe) and high odor discrimination (83.3%) and identification (97.5%) accuracies. Both molecular dynamics simulations (MDS) and density functional theory (DFT) were employed to elucidate the adsorption interaction between odorant molecules and sensing materials. Our work demonstrates that the developed e-olfaction exhibits excellent olfactory performance in sniffing out VOC-based odors. This work could facilitate miniaturization of e-noses, digitization of odors, and distinction of volatile organic compounds (VOCs) in various emerging applications, such as molecular discrimination, food quality identification, disease diagnosis, etc.

## References

- [1] Shirong Huang, et al. Applied Physics Reviews 10.2 (2023).
- [2] Parichenko, Alexandra, et al. TrAC Trends in Analytical Chemistry (2023): 117185.
- [3] Shirong Huang, et al. Advanced Intelligent Systems 4.4 (2022): 2200016.
- [4] Li, Yufen, et al. Small 19.14 (2023): 2206126.
- [5] Shirong Huang, et al. Carbon 173 (2021): 262-270.

## Figures



**Figure 1:** Odor classification results by Linear Discriminant Analysis (LDA) classifier algorithm in 3D space.