Machine Learning-enabled Biomimetic Electronic Olfaction Using Graphene Single-channel Sensors

Shirong Huang
Institute for Materials Science and
Max Bergmann Center for Biomaterials
TU Dresden
Dresden, Germany
shirong.huang@tu-dresden.de

Alexander Croy
Institute for Physical Chemistry
Friedrich Schiller University Jena
Jena, Germany
alexander.croy@uni-jena.de

Antonie Bierling
Department of Psychotherapy and
Psychosomatic Medicine
TU Dresden
Dresden, Germany
antonie.bierling@tu-dresden.de

Luis Antonio Panes-Ruiz
Institute for Materials Science and
Max Bergmann Center for Biomaterials
TU Dresden
Dresden, Germany
luis_antonio.panes_ruiz@tu-dresden.de

Bergoi Ibarlucea
Institute for Materials Science and
Max Bergmann Center for Biomaterials
TU Dresden
Dresden, Germany
bergoi.ibarlucea@tu-dresden.de

Gianaurelio Cuniberti
Institute for Materials Science and
Max Bergmann Center for Biomaterials
TU Dresden
Dresden, Germany
gianaurelio.cuniberti@tu-dresden.de

Abstract—**Olfaction is an evolutionary old sensory system, yet it provides sophisticated access to information about our surroundings. Inspired by the biological example, electronic noses (e-noses) in combination with efficient machine learning techniques aim to achieve similar performance and thus digitize the sense of smell. Despite the significant progress of e-noses, their development remains challenging due to the complex layout design of sensor arrays with a multitude of receptor types or sensor materials, and the need for high working temperature. In the current work, we present the discriminative recognition of odors utilizing graphene single-channel nanosensor-based electronic olfaction in conjunction with machine learning techniques. Multiple transient features extracted from the sensing response profile are employed to represent each odor and used as a fingerprint of odors. The developed electronic olfaction prototype exhibits excellent odor identification performance at room temperature, maximizing the obtained results from a single nanosensor. The developed platform may facilitate miniaturization of e-nose systems, digitization of odors, and distinction of volatile organic compounds (VOCs) in various emerging applications.**

Keywords—Olfaction, e-nose, odor identification, graphene

I. Introduction

Human sensation relies on the sensory organs, such as eyes, ears, skin, tongue, and nose, which contribute to the sensory perceptions of vision, audition, somatosensory, gustation, and olfaction in the brain, respectively. Thanks to the surging development of artificial intelligence technology, there are numerous well-established technologies for measuring and reproducing some of the human senses, for instance, computer vision mimicking human sight, [1-3] machine audition mimicking human hearing, [4, 5] electronic skins mimicking human skins, [6-8] while it has proved more challenging to mimic the sense of taste and smell since they are chemical senses and responsive to chemical stimuli. [9] Nevertheless, olfaction, as one of the oldest senses in terms of evolution, is one of the most effective ways of interacting with the environment. In order to provide olfactory information and process odors artificially, machine olfaction gives rise to developments in biological modeling, sensor technology, and bioinspired technologies. In this scenario, machine olfaction or electronic nose (e-nose), refers to instrumental replication of the human olfactory sense, which comprises an array of electronic chemical sensors with partial specificity and an appropriate pattern-recognition system, capable of recognizing simple or complex odors, as defined by Gardner and Bartlett in 1993. [10]

Herein, we present the development of a highly discriminative and ultrasensitive electronic olfaction (e-olfaction) platform for the detection, discrimination, and identification of basic odor molecules, based on the use of a single channel nanosensor utilizing non-covalently functionalized graphene as a sensing element material. Four odors, including eucalyptol (Euca), 2-nonanone (2Nona), eugenol (Euge), and 2-phenylethanol (2Phe), which are generally employed in olfactory training among patients with olfactory loss, were investigated in this work. The performance of the developed e-olfaction towards individual odors is evaluated *via* machine learning algorithms incorporating 11 transient features extracted from the characteristic sensing response profile. The machine learning techniques involve data processing of sensing response, dimensionality reduction of features, as well as training classifier algorithms for odor prediction. The developed platform allows for odor recognition of a wide spectrum of molecules toward assisted olfaction for the population who exhibit olfactory disorders, as well as detection of volatile organic compounds (VOCs) in an extensive variety of domains, e.g., environmental monitoring, public security, smart farming, or disease diagnosis (e.g., lung cancer, COVID-19).

II. Results and Discussions

In the presence of odor labels, the odor identification performance of our e-olfaction platform was investigated, corresponding to a supervised machine learning approach. This technique utilizes labeled datasets to train algorithms for the classification or the prediction of outcomes for unknown datasets accurately. The dataset (Euca, 2Nona, Euge, 2Phe, and reference gas), as well as their label were processed by the classifier model. We used Linear Discriminant Analysis (LDA) as an example, which is a linear transformation technique for dimensionality reduction and a well-known classifier. Odor classification results are illustrated in Figure 1 (a)-(b). The first three linear discriminants account for the total variance (LD1, LD2, LD3 explain 82.42%, 14.36%, 2.67% of the variance, respectively). These results suggest that the four odor clusters as well as the reference cluster are separated very well without overlapping. With a 10-fold cross-validation

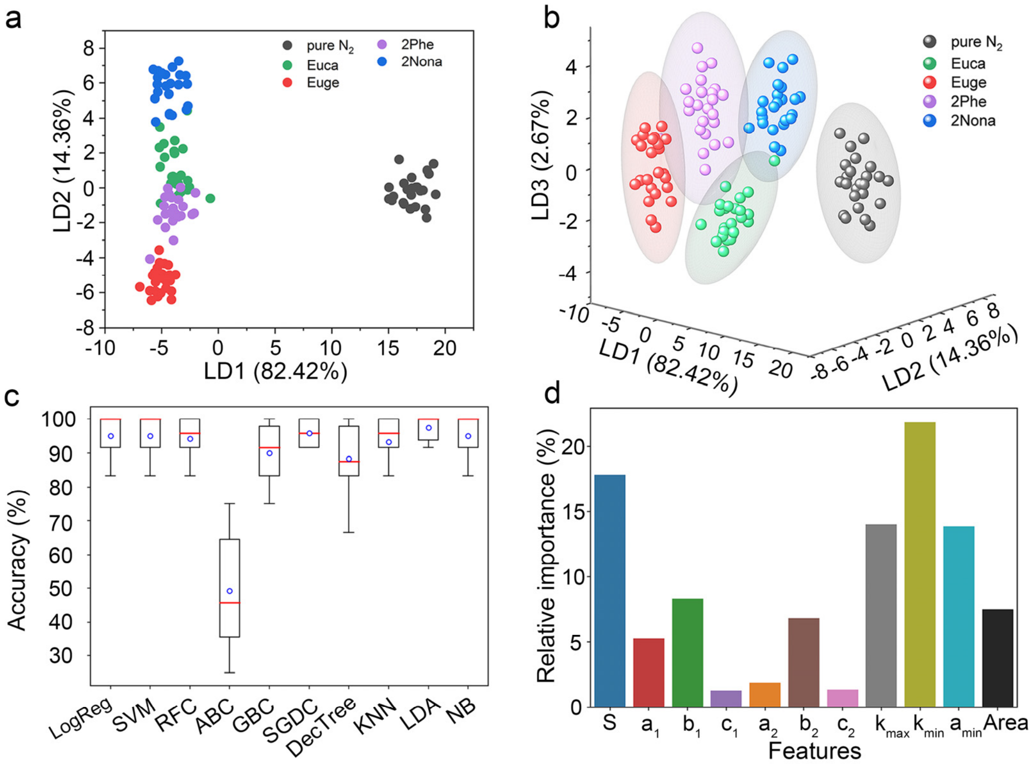

Figure 1. Odor identification performance of the e-olfaction platform. (a) Odor classification results by Linear Discriminant Analysis (LDA) classifier algorithm in 2D space (LD1 vs LD2). (b) Odor classification results by LDA classifier algorithm in 3D space (LD1 vs LD2 vs LD3). (c) Average prediction performance using 10-fold cross-validation on various algorithms. (d) Relative importance loading of 11 features on the odors identification.

approach, the average classification accuracy was evaluated with respect to various classifier models, as shown in Figure 1 (c). For most classifier models, the prediction accuracy is very high, particularly, implemented with the LDA classifier, the accuracy reaches 97.5%.

To evaluate the contribution of odor features to odor identification, the importance weight of these 11 feature parameters (a_1, b_1, c_1, a_2, b_2, c_2, S, k_{max}, k_{min}, a_{min}, $Area$) were analyzed using the RandomForest classifier algorithm. As depicted in Figure 1 (d), it is observed that the most important 4 features (S, k_{max}, k_{min}, a_{min}) parameters make up 57.9% of total feature importance and the sole feature k_{min} contributes to 21.4% of total feature importance. These results indicate that the transient derivative features (S, k_{max}, k_{min}, a_{min}) are discriminative for different odors.

In conclusion, a biomimetic electronic olfaction platform using a graphene single-channel nanosensor has been proposed and its performance at room temperature has been investigated. Based on the preliminary results, the developed e-olfaction platform exhibit excellent odor identification performance. The developed e-olfaction device could be applied for the detection and discrimination of volatile organic compounds in widely emerging fields.

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