

## Mendeleev 2024

XIII International Conference on Chemistry for Young Scientists

# BOOK OF ABSTRACTS



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## XIII International Conference on Chemistry for Young Scientists "MENDELEEV 2024"

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#### NANOCOMPOSITES WITH CHARGE TRANSFER FOR RECOGNITION ORGANIC MOLECULES IN GAS PHASE BASED ON PHOTOCATALYSIS

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Recognition of organic molecules in the gas phase using compact and inexpensive devices is an important task in modern technologies. Living organisms solve this problem through biochemical reactions on olfactory receptors, providing unprecedented selectivity, which underlies odor recognition. In engineering, this task is addressed using semiconductor gas sensors based on metal oxides. However, the reaction of oxidation of organic molecules by chemisorbed oxygen, which is the basis of their operation, requires high temperatures and has low selectivity, fundamentally limiting the use of gas sensors. This study proposes a new concept for the operation of a gas sensor using photocatalysis on quantum dots (QDs) with photoexcited electrons transfer to the transport matrix of oxide semiconductor, resembling olfactory receptors.

In this work, hybrid nanocomposites based on CdSe QDs with organic ligands and nanodispersed powders of SnO<sub>2</sub> were studied. The photooxidation of aliphatic alcohols was chosen as a model reaction for photocathalysis. This is the reaction that does not require oxygen, oxidants, or heating, which are commonly used in the oxidation by chemisorbed oxygen in traditional gas sensors. CdSe QDs were synthesized using a colloidal method and the size of QDs was controlled with the time of the synthesis and optical spectroscopy. Native long-chain oleic acid ligands on the surface of CdSe QDs were exchanged for a series of short-chain molecules containing a thiol group for binding to the CdSe surface and a carboxyl group for binding to the metal oxide surface. The photocatalyst was obtained by immobilizing and chemically binding CdSe QDs on the surface of the ultra-dispersed metal oxide matrix. Photochemical reactions occurring on the system's surface were detected by monitoring the electrical resistance of the oxide matrix. The interaction of the photocatalyst surface with the gas phase was studied using methanol, ethanol, butanol-2, acetone, acetic acid, ethanal, methanal as examples. Device prototypes were fabricated by applying the photocatalyst to microelectronic chips to control electrical resistance. The photocatalytic reaction was provided under the yellow radiation with a wavelength of 595 nm. SnO<sub>2</sub> samples modified with QDs have lower baseline resistance than pure samples of SnO<sub>2</sub> due to electron transfer from QDs to the oxide matrix. An increased resistance amplitude is observed after introducing 100-1000 ppm of the analyzed organic molecule in gas phase compared to an inert atmosphere, attributed to the interaction of the photoexcited hole with alcohol molecules. Concentration dependence on different organic compounds ratios was also investigated. The sensor response dependency on the distance between QDs and the metal oxide matrix was studied by varying the length of the organic ligand chain, as well as evaluating the influence of ligand coordination (carboxylate and thiolate). The process of photooxidation of organic molecules by photocatalysts was established with a detailed analysis of photocatalysis products using FTIR, DRIFT, and NMR spectroscopy.

#### References

[1] Science **2014**, 343, 1370

[2] The Journal of Physical Chemistry Letters 2021, 12, 7180

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