

Titolo:

FT-IR spectroscopy coupled with machine learning for a high sensitive detection and discrimination of gaseous volatile organic compounds.

Authors

Macis S., D'Arco A., Paolozzi M., Mancini T., Mosesso L., Paolozzi M. C., Marcelli A., Radica F., Tranfo G., Della Ventura G., Tamascelli S., Lupi S.

Volatile Organic Compounds (VOCs), such as styrene and its co-products, are organic chemical compounds able to evaporate at room temperature. They are classified as a possible human carcinogen in the short and long term and in co-exposure to other physical-chemical agents. During the last years, we systematically used Fourier Transform Infrared (FTIR) spectroscopy for quantifying VOCs in air, increasing the sensitivity of IR systems down to the parts per million (ppm) level. Here, we investigate five selected aromatic compounds, of extreme importance in occupational safety with the aim of filling the gap in IR gas-phase database. Benzene, Toluene, and Xylene (BTXs) are studied and their calibration curves are carried out. A Machine Learning (ML) algorithm is developed, providing the automatization of the single VOC detection and discrimination starting from the spectra of random mixtures. The dataset processing is optimized and different algorithms are evaluated over each single VOC recognition between styrene, ethanol, isopropanol, acetone, and BTXs. This work is a very promising starting point for building a portable setup for the detection at very high sensitivity.

speaker:

Dr. Salvatore Macis

Researcher at Sapienza Terahertz Laboratory

Sapienza University of Rome, Piazzale Aldo Moro, 5, 00185 Rome, Italy

