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DOCTOR OF ENGINEERING SCIENCES

of **Thomas Virdis**

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METAL-ORGANIC FRAMEWORKS AS SELECTIVE ADSORPTIVE MATERIALS FOR DETECTION OF FOOD-SPOILAGE INDICATORS: CHALLENGES AND OPPORTUNITIES

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Abstract of the PhD research

In the EU, 33 million people cannot afford a quality meal every second day, and each person is responsible for approximately 180 kg of food waste every year. At the current growth pace of our society, food loss and waste has become a compelling problem which consequences will be unbearable in the coming future. These problems can be alleviated by developing new smart packaging strategies, envisaging the use of dedicated sensors aimed at real-time food quality monitoring and spoilage recognition.

The detection of volatile organic compounds (VOCs) present in the headspace of food packages provides a crucial insight on the quality of the food products, allowing for reliable recognition of any spoilage processes ongoing. The identification and quantification of these molecules is very challenging due to their ultra-low concentrations, the immense diversity of the VOCs released during shelf-life and the very high humidity inside the food packaging. Industries of the food supply chain and food retailers have pushed researchers to seek new strategies aimed at rapid and reliable VOCs detection in food packages, to eventually manufacture integrated sensors for food quality monitoring in real time. Such microdevices could be developed using adsorptive coatings that selectively trap molecules pointing at food spoilage. These adsorptive coatings are coupled to an integrated optical component that, upon stimulation through an external light source, can return a measurable signal straightforwardly linked to the concentration of specific food spoilage associated molecules.

This strategy for microsensor development was proposed in the frame of the SBO-funded project Check Pack (2013-2017). The research carried out in this PhD focused on the study of the adsorption properties for multiple combinations of Metal-Organic Frameworks as adsorbents and approximately 20 volatile food spoilage indicators. Physical properties of the adsorbents were investigated by means of Ar porosimetry and N_2 sorption. Gravimetric analysis and vapor adsorption breakthrough experiments have been performed to measure the single-component adsorption isotherms of chosen VOCs at 25 °C and 6 °C, mimicking the conditions of the environment enclosed within the food packages, which compels high-complexity vapors mixtures at generally low concentration and high relative humidity (≈ 90%). The thermodynamic properties at infinite dilution were studied through Pulse Gas Chromatography, which allowed calculating the enrichment factors for different adsorbents at 25 °C and 6 °C. Furthermore, an innovative approach based on Selected Ions Flow Tube Mass Spectrometry has been developed, to study adsorption dynamics with multi-component breakthrough experiments at ultra-low concentration. Eventually, we propose a proof-of-concept for fluorescence-based molecular recognition by means of Luminescent Metal-Organic Frameworks with fluorescent properties, discussing the effect of guest uptake on the resulting emission of the system in regards to their potential future application in the VOC sensing frame.