QUANTUM TECHNOLOGIES, METAMATERIALS, AND THE FUTURE OF CB SENSING

First-principles Analysis of Transition Metal Nitrates in oxide Host Sensor Materials

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The warfighter is often tasked with the responsibility of investigating possible rogue laboratories, searching for materials that can be used to build or develop weapons that can range from improvised explosive devices to chemical warfare agents for direct attack. Currently, the warfighter's primary method of chemical detection comes in the form of colorimetric paper. It is a mid-20th century technology that comes in the form of a paper detection system that, like litmus, changes color according to the reagent detected. This method doesn't come without its limitations. It can be subject to false alarms to some common non-toxic organic compounds, and the color changes that occur don't always match with the legend that is provided. Many of the chemical detection systems of the twenty-first century involve technological advancements involving techniques from Raman spectroscopy to thin layered reaction systems that use graphene. Raman spectrometers, while man-portable and capable of providing specific molecular fingerprint information, may still be bulky and can add a significant weight for the warfighter to carry. Conversely, graphene-based systems can be used in convenient handheld and wearable devices and provide great sensitivity; however, as they respond to a wide range of molecules, their selectivity becomes limited and they can be susceptible to rapid aging and damage from atmospheric exposure. This work aims to provide a convenient, reliable and, cost-efficient alternative to current detection methods, while allowing for a wider range of chemical activity. Preliminary work with inorganic oxides, such as zeolites, have shown promise as a colorimetric sensor with the potential to be as portable as graphene while providing greater selectivity and more chemical information in the form of specific color changes. The aluminosilicate zeolite explored uses a hydrogen counter-ion and is composed of corner sharing Si/Al tetrahedrons, allowing for multiple bonding orientations which produce a 3D framework of multiple pores of various sizes as well as producing various polytypes. By exposing various metal nitrates to these aluminosilicate zeolites, color changes have been noted. Using density functional theory, we can model these metal nitrate and zeolite interactions. This multifaceted work will explore the structural nature of the aluminosilicate zeolite being explored, the adsorptive interactions that occur between the zeolite and the metal nitrates and determine the spectroscopic changes that occur as a result of these interactions. Modelling the transition metal and zeolite interactions, along with the calculation of the electronic band structures of these materials will give us insight into the light absorbing nature of these combinations, allowing us to determine the nature of the color change observed.

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