Unveiling the Potential of $Ti_3C_2X_2$ (X = O, S) MXenes for 3-Hydroxy-2-Butanone Detection: A Promising Sensor for Lung Cancer Biomarkers

Somratchanee Puarsa,[1] and Thanayut Kaewmaraya*[1]

[1] *Department of Physics, Faculty of Science, Khon Kaen University, Khon Kaen, Thailand;*
Email: thakaew@kku.ac.th

Lung cancer has been ranked among the most prevalent cancers and contributing to high mortality rates worldwide. Breath analysis has emerged as an innovative, non-invasive diagnostic technique for early-stage detection, enabling timely intervention before the disease progresses to more severe stages. However, effective breath analysis requires highly sensitive and selective gas sensors. In this study, we explore the potential of two-dimensional (2D) $Ti_3C_2X_2$ MXenes (X = O, S) as room-temperature sensors for detecting 3-hydroxy-2-butanone (3H-2B), a volatile biomarker associated with lung cancer metabolism. Using density functional theory (DFT) calculations and thermodynamic analysis, we investigate key gas-sensing parameters, including binding energy, electronic properties, charge transfer, bonding interactions, sensing coverages, and recovery times. Our results reveal that $Ti_3C_2O_2$ MXene exhibits stronger binding energy compared to $Ti_3C_2S_2$, enhancing its adsorption capabilities and making it a more efficient candidate for 3H-2B detection. Additionally, both materials demonstrate high sensitivity and selectivity toward 3H-2B, indicating their potential for accurate and reliable lung cancer diagnostics.