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PhD Dissertation Defense

Entitled

AB-INITIO INVESTIGATION OF TRANSITION METAL DICHALCOGENIDE MONOLAYER FOR OPTOELECTRONIC, GAS-SENSING, INFORMATION- AND ENERGY-STORAGE APPLICATIONS

by

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Date & Venue

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Abstract

The research focuses on Transition Metal Dichalcogenide Monolayers (TMD-MLs), a unique class of 2D materials known for their outstanding properties. These properties position them as promising candidates for various applications. This study primarily concentrates on the use of TMD-MLs for these applications, in addition to the exploration of MXene ($Ti_3C_2T_x$) for the detection of lung cancer biomarkers. To ensure accuracy, the research employs two computational methods: VASP for electronic and magnetic properties and ATK for large system transport properties.

1. In the realm of **Optoelectronics**, TMD-MLs offer opportunities for advanced light control technologies. The study delves into band gap engineering, crucial for controlling intrinsic band gaps and optimizing device performance. Investigating various alloys, the research identifies the dependency of the band gap on the metal ratio, emphasizing the significance of the Mo/W ratio in bandgap engineering applications.
2. In the field of **Information Storage**, utilizing spin as a quantum feature of electrons enables the providence of half-metallicity in accommodating materials. Through computational methods, the study investigates defective TMD monolayers and transition-metal doped TMDs. The results highlight the critical distance for ferromagnetic-coupling interactions, crucial for the existence of half-metallicity, thus, providing essential insights for spintronics applications.
3. In the field of **Energy Storage**, the research explores the challenge of safe hydrogen storage. Several substrates based on doped $MoSe_2$ monolayers and $MoSe_2$/graphene bilayers are studied for their potential in hydrogen storage. Specific doping (e.g., Mn, Ni, and Cu) enhances the materials' hydrogen uptake capacity, showcasing their potential as candidates for safe hydrogen storage systems.
4. In the field of **Gas Sensing**, the study investigates toxic nitrogen-containing gases' adsorption and gas-sensing properties on transition metals functionalized MoS_2 monolayers. The results demonstrate promising sensor responses due to changes in magnetic states, presenting a significant advancement in gas sensing technologies.
5. In the field of **Lung Cancer Diagnosis**, the research explores $Ti_3C_2T_X$ MXenes and doped TMD-MLs for biomarker detection. Functionalized MXenes show selective detection of volatile organic compounds (VOCs), making them suitable candidates for early lung cancer diagnosis. Additionally, TMD-MLs doped with specific transition metals exhibit enhanced surface polarity, enhancing their suitability as biosensors for lung cancer biomarker detection.

Keywords: 2D materials, Optoelectronics, Gas-sensing, Spintronics, Hydrogen storage, Early diagnosis of Lung cancer, Volatile organic compounds (VOCs) biomarkers, DFT.