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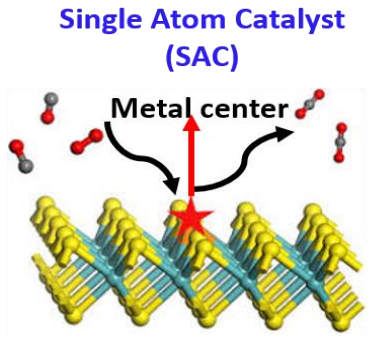
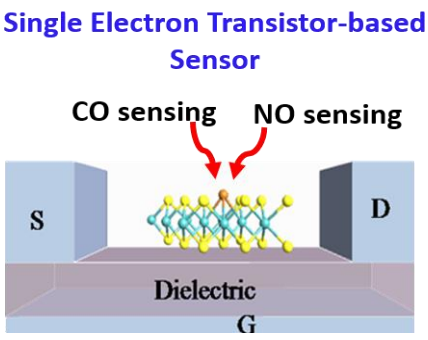
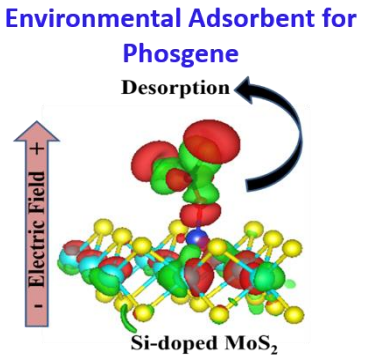
Title of the Thesis:	*Computational Study of Functionalized MoS_2 for Environmental and Energy Applications*

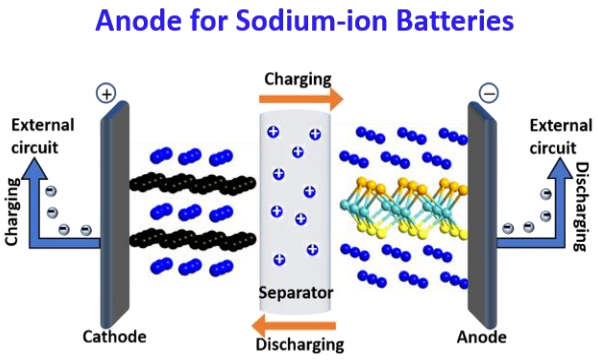
Abstract

In this thesis, functionalized form of 2D material, MoS_2, is studied computationally for environmental and energy applications in Density Functional Theory (DFT) framework with an aim to (1) exploit the advanced modern computational tools for the prediction of materials' properties and to gain atomic-level insights into the adsorption and decontamination phenomena as well as electrochemical performance, (2) simulate and understand the implications of functionalization of monolayer MoS_2 with cost-effective materials in terms of binding energy, electronic structure, thermal stability, and (3) further investigate them as a single atom catalyst, single electron transistor (SET)-based sensor, environmental adsorbent and anode material for sodium-ion batteries.









In environmental domain, I have computationally studied economical single atom catalysts (SACs) with MoS_2 supported single Cu and Mo for CO oxidation, single electron transistor (SET) based CO/NO sensor with Cu-doped MoS_2 as an island and Si-doped MoS_2 as environmental adsorbent for phosgene molecule. All the proposed functionalized MoS_2 structures are found to be thermally stable as evident from *ab initio* molecular dynamics (AIMD) calculations. CO oxidation catalysis of proposed SACs suggests that O_2 molecule is strongly activated by both Cu and Mo metal center which prevents CO accumulation and hence avoids poisoning of the catalysts. The minimum energy paths (MEPs) are investigated further using climbing image-nudged elastic band (CI-NEB) method and diffusion barriers are calculated. In terms of reaction kinetics, Cu-doped MoS_2 has been predicted to offer far better performance than Mo_S-doped MoS_2. Thermal corrections are considered by calculating Gibb's Free energy at room temperature which gives low energy barrier and fast reaction rate for Cu-embedded MoS_2.

Single electron transistor-based sensor with Cu-doped MoS_2 as an island is proposed as futuristic low-powered, gate-controlled CO and NO gas sensor with better sensing characteristics than pristine MoS_2. It shows better sensitivity due to increase in number of charge states at a given bias and gives better response due to reduction in charging energy and hence blockade voltage. Also, detection of CO and NO gas molecules at different gate bias leads to their easy identification.

Si-doped MoS_2 is proposed as an effective environmental adsorbent for phosgene gas molecule due to their strong interaction which results in modulation of energy band gap and work function of the material. Further it is found that a perpendicular electric field promotes complete desorption of phosgene molecule at 0.6 V/Å, which reactivates it for recycling. Such bond weakening is explained in terms of charge transfer and dipole moment variations.

For energy storage application, alloy of MoS_2 and $MoSe_2$ is utilized as a potential anode material for rechargeable sodium-ion batteries (SIBs). Introduction of selenium boosts the conductivity, mechanical strength and structural stability of MoS_2 monolayer. Fast diffusion kinetics is predicted in terms of low diffusion barrier. Very importantly, it demonstrates that the alloy can withstand large strains without breaking attributed to the maximum lattice expansion (6.08%) lying in the range of bearable strain limit (24%).

Keywords: *MoS_2, DFT, Catalysis, SET, Sensor, Phosgene, Batteries.*