ABSTRACT

To manipulate the physical properties such as optical, electronic, transport and magnetic properties of TMDs for diverse technological applications, researchers have demonstrated that substitutional or interstitial doping with alternative transition metal ions can be effectively utilized and it could be beneficial to various applications. In light of the above, the present study meticulously investigates the effects of cobalt doping in Mo site of MoS_2 nanostructure. Hence motivated by these facts, MoS_2 nanostructures in the form of nanosheets and nanoflowers have been synthesized with systematic doping of Co-ion (2% Co, 4% Co, 8% Co) by utilising one-step hydrothermal synthesis route. Such doping of Co-ion in MoS_2 nanoflakes introduces catalytically active edge sites, metallic 1T-edges, defective basal planes and among them 6% Co- MoS_2 nanosheets exhibited highest catalytic activity towards reduction of harmful nitroarene (p-nitrophenol). Hence, in this thesis it is well demonstrated that proper tuning of Co doping in MoS_2 nanosheets paves the way in searching for a potential alternative of a noble metal catalyst for the catalytic reduction of nitroarenes. In addition, such kind of doping contributes to the i) enhanced ferromagnetism (ferromagnetic coupling on the scale of $p_{eff} \sim 4.37\ \mu_B$) ii) improved transport properties iii) tunable temperature coefficient of resistance (TCR) $\sim 3.0 \times 10^{-2}\ K^{-1}$. Interplay of various transport models (variable range hopping, nearest neighbour hopping) within different temperature regime have been evidenced in Co-doped MoS_2 systems. Therefore, our approach in achieving mixed-phase defect-rich (1T and 2H) Co-doped MoS_2 NFs exhibiting room-temperature ferromagnetism, high TCR makes them an excellent multifunctional candidate in spintronics, infrared (IR) detection.

However, annealing of Co-doped MoS_2 nanosheets at high temperature (800 °C) in vacuum can introduce a few exotic things such as improved crystallinity, the larger crystallite size (from

diffused grain to discrete grain) and lesser grain boundaries leading to lesser defects are considered to be efficient in designing excitonic devices for delivering longer charge carrier time and less recombination. Our findings establish that cobalt doping in layered TMD materials with high-temperature vacuum annealing conditions enables controlled tuning over exciton dynamics, enhancement in charge carrier relaxation rate upto one order and regulated defect-assisted carrier relaxation rate. Control over such excitonic properties facilitates the efficient design of exciton-based optoelectronic devices in the future.

Composite of MoS_2 with other conducting materials such as PANI has been proved to enhance the electrochemical properties effectively by providing large number of active sites for electrochemical reaction, and the gaps between oriented PANI nanowires can serve as ion channels for fast electrolyte transport as well as accommodate the large volume changes. Herein, PANI/MoS_2 composite heterostructure have been synthesized utilising chemical polymerization method in presence of L-ascorbic acid (L-AA). L-AA are able to form self-assembly of their rod-like structure through H-bonding which leads to successful growth of PANI nanotubes on MoS_2 templates. The optimized PANI-/1T@2H MoS_2 hybrid functionalised with L-ascorbic acid (L-AA), denoted as PM2, delivers a high specific capacitance of 618 F/g at a current density of 1 A/g and a good rate retention up to 73% with the increase in current density from 1 A/g to 10 A/g in a three-electrode system. Interestingly, the symmetric supercapacitor (SSC) integrated using PM2 hybrid delivers efficient capacitive property (160 F/g at 0.3 A/g), energy, and power density (8 Wh/kg and 6.1 kW/kg). It has been evidenced that PM2 hybrid exhibits excellent electrochemical properties as a supercapacitor electrode material, having capacitive retention up to 98.1% even after completing 8000 cycles at a current density of 2 A/g. Additionally, PM2 SSCs possess an excellent degree of mechanical properties and flexibility, and they are able to power a red LED successfully when connected in series. Our strategy of growing PANI onto L-AA functionalized 1T@2H MoS_2

provides a possible pathway to enhance the electrochemical performance of PANI/MoS_2-based hybrid materials for the design of future-generation energy storage devices.

Keywords: Transition metal dichalcogenides, MoS_2, nanosheets, catalyst, relaxation rate, polyaniline, supercapacitors, capacitance, cycling stability, electrochemical performance.