INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Exploring Charge Storage Mechanism in MXene as Supercapacitor Electrode: A First-Principles Approach

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SHORT ABSTRACT

The exfoliation of layered transition metal carbides/nitrides, MXenes ($M_{n+1}X_n$), from its 3D precursor MAX is remarkable event in the history of 2D materials. Ti_3C_2 , the first discovered MXene, caught everyone's attention due to its excellent charge storage capacity as a supercapacitor electrode. It has been the most explored MXene in this 2D subfamily. 70% of the MXene research is on this compound only. Baring Ti_3C_2 , various other transition metal-based MXenes have been synthesized to date. This 2D subfamily exhibits diversity in structure and composition. MXene is enormously famous due to its performance as an energy storage device. The high electrical conductivity, hydrophilicity, surface redox activity, and mechanical stiffness make it a potential alternative to Graphene as an electrode in energy storage devices like batteries and supercapacitors. Experimental evidence suggests that diversity in structure, composition, and surface passivations affect the supercapacitive property of MXenes. However, there are a few scattered attempts to explore these aspects for varieties of systems to understand the mechanisms of charge storage in MXene-based supercapacitors. This thesis provides a systematic study on understanding structural and compositional effects on the electrochemical performances of MXene-based supercapacitors. Our investigations start with exploring the capacities of M 2 C and M 3 C 2 MXenes as supercapacitor electrodes. We consciously choose various 3d and 4d transition metals as M elements. We show the significance of quantum capacitance on energy storage performance. We also explain the effect of surface passivation on MXene capacitances. Further, we provide a comparative study of substitution and doping in enhancing the storage capacity of MXenes. An explanation of the influence of doping sites on the redox capacitance of Ti 3 C 2 is given. Next, we attempt the route of surface engineering to improve the energy storage capacities of MXenes. To this end, we construct Janus MM'C MXene and study their electrochemical performances. In the course of this study, we find that much superior capacities are obtained if one of the components of Janus is a magnetic element. We extend the study by considering solid solutions of one of these systems and investigating the effect of chemical and magnetic disorders on its supercapacitive performance.

In a nutshell, this thesis systematically explores the structure-property relationships about electrochemical performances of various MXenes that can yield substantial insights into the physics and chemistry of this family of 2D compounds.