Design of 2D Material-Based Heterostructures for Rechargeable Batteries

A thesis presented for the award of the degree of

Doctor of Philosophy

from

University of Technology Sydney

By

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CERTIFICATE OF ORIGINAL AUTHORSHIP

I, *Shijian Wang* declare that this thesis, is submitted in fulfilment of the requirements for the award of *Doctor of Philosophy*, in the *School of Mathematics and Physical Sciences, Faculty of Science* at the University of Technology Sydney.

This thesis is wholly my own work unless otherwise referenced or acknowledged. In addition, I certify that all information sources and literature used are indicated in the thesis.

This document has not been submitted for qualifications at any other academic institution.

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DEDICATION

This thesis is dedicated to my family and my beloved scientific career.

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LIST OF PUBLICATIONS

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ABSTRACT

Two-dimensional (2D) materials have been regarded as promising electrode materials for rechargeable batteries because of their advantages in providing ample active sites and improving electrochemical reaction kinetics. However, it remains great challenges for 2D materials to fulfill all requirements for high-performance energy storage devices in terms of electronic conductivity, the number of accessible active sites, structural stability, and mass production capability. Recent advances in constructing 2D material-based heterostructures offer opportunities for utilizing synergistic effects between the individual blocks to achieve optimized properties and enhanced performance for rechargeable batteries. In this doctoral thesis, several 2D material-based heterostructures varying from 0D-2D, 1D-2D to 2D-2D heterostructures have been designed, synthesized, and applied to rechargeable batteries. These include Sb single atoms and quantum dots co-decorated $Ti_3C_2T_x$ MXene-based aerogels (0D-2D heterostructure), N-doped conductive carbon coating and 2D graphene nanosheets co-modified Sb_2Se_3 nanorods (1D-2D heterostructure), and superlattice-like 2D-2D heterostructure constructed by unilamellar MnO_2 and graphene nanosheets. The specific morphology features, physicochemical properties of these heterostructures, and their functions on ion storage mechanisms and kinetics have also been deeply investigated. The enlightening techniques in this thesis provide promising design strategies for 2D material-based heterostructure electrodes in rechargeable batteries.