Transition metal dichalcogenides films for photo-driven water splitting

Introduction

Two-dimensional (2D) transition metal dichalcogenides (TMDs) with lamellar structures similar to that of graphite have received significant attention because of their favorable properties such as sizable bandgaps, tunable carrier type (n- or p-type) as well as its earth abundance.[1] In addition, the tunable electronic structure of TMDs make them attractive for a variety of applications as chemically active electrocatalysts for hydrogen evolution and hydrosulfurization, as well as electrically active materials in opto-electronics. In particular, the semiconducting chalcogenides MoX₂ and WX₂ (X=S or Se) show tunable band gap characteristics corresponding to the number of layers. Remarkably, WSe₂ based photovoltaic (PV) and photoelectrochemical (PEC) devices achieved 8.6 and 14% energy conversion efficiency, respectively.[2] To take advantage of the 2D nature of TMDs in PEC applications, we adopt ultrasonic exfoliation to fabricate thin WX₂(X=S, Se). The exfoliated WX₂(X=S, Se) dispersed in organic solvents is then deposited on FTO glass via an electrophoretic deposition technique. Post-treatment such as thermal annealing to improve film quality will be done in a home-build thermal chemical vapor deposition (CVD) system. The as-prepared WX₂(X=S, Se) films will be evaluated for electrochemical as well as photoelectrochemical hydrogen evolution reaction (HER).

Project objectives

The present project will focus on exfoliation of bulk WX₂(X=S, Se) via ultrasonication and subsequent film preparation by electrophoresis. In particular, the following important aspects of the process need to be investigated:

1) Optimized exfoliation (ultrasonication) parameters (solvents, sonication power, time, etc.) should be reached, TEM tests will be done to evaluate the exfoliated WX₂(X=S, Se).
2) Electrophoresis technique will be applied for film preparation.
3) Film quality will be evaluated by various techniques such as XRD, Raman, SEM, UV-VIS spectroscopy.
4) Electrochemical and photoelectrochemical tests of hydrogen evolution activity.


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