Exploring Atomic Layers for Photocatalysis

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Abstract

Two-dimensional (2D) layered materials exhibit exceptional properties, such as high carrier mobility, wide range of light absorption/emission and relatively narrower band gap, which make them ideal candidates for the construction of novel photocatalysts[1]. 2D layered semiconductors, such as semiconducting transition metal dichalcogenides (STMDs) are the new members of 2D materials family that consist of a "sandwich" structure of a transition metal layer (e.g. M: Mo, W) covalently bonded between two chalcogen layers (e.g. X: S, Se, Te) to form MX2: MoS_2, WS_2 etc. They have gained worldwide attention in recent years. Engineering various combinations of STMDs based on stacking sequence, alloying and crystal phase will provide unique opportunities to tailor new -dedicated materials for different applications.[2-3] Vertical/lateral vdW STMDs heterostructures have attracted considerable research interest due to their efficient electron-hole separation during the conversion of light to current, and these have found use in high- performance optoelectronic devices and photocatalysts. In this talk, I demonstrate the fabrication and characterization of MoS_2 and WS_2 based atomic layers and their alloyed versions withof 'Se' ($MoS_{2(1-x)}Se_{2x}$, $WS_{2(1-x)}Se_{2x}$). Morphology and crystalline quality of alloys are assessed using Raman and X-ray photoelectron spectroscopy. In particular, homogeneity of layers (mono and few layers) and alloying of Se over mono and few layer MoS_2 and WS_2 are estimated from HAADF-STEM imaging. In addition, I will present density functional theory calculations in order to estimate the charge density distribution between S and Se on the MoS_2 basal plane, which shows S in the Se environment has higher charge density compared to S without Se which makes it active towards hydrogen evolution reaction (HER) activity.

References

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Figures

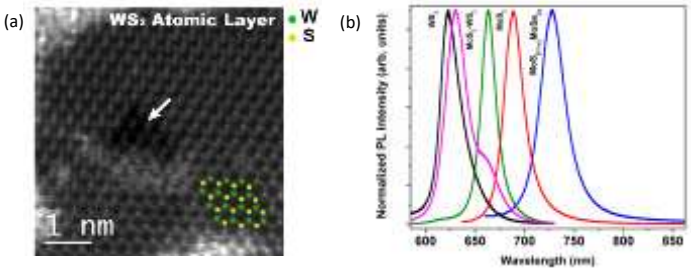

Figure 1: (a) Atomic resolution HAADF STEM image of single layer WS2 and an arrow indicates a S vacancy. (b) Tunable photoluminescence from MoS_2, WS_2 based vdW STMDs