Atomic-Level Customization of 4 in. Transition Metal Dichalcogenide Multilayer Alloys for Industrial Applications - DTU Orbit (18/10/2019)

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Despite many encouraging properties of transition metal dichalcogenides (TMDs), a central challenge in the realm of industrial applications based on TMD materials is to connect the large-scale synthesis and reproducible production of highly crystalline TMD materials. Here, the primary aim is to resolve simultaneously the two inversely related issues through the synthesis of MoS2(1- x ) Se2 x ternary alloys with customizable bichalcogen atomic (S and Se) ratio via atomic-level substitution combined with a solution-based large-area compatible approach. The relative concentration of bichalcogen atoms in the 2D alloy can be effectively modulated by altering the selenization temperature, resulting in 4 in. scale production of MoS1.62 Se0.38 , MoS1.37 Se0.63 , MoS1.15 Se0.85 , and MoS0.46 Se1.54 alloys, as well as MoS2 and MoSe2 . Comprehensive spectroscopic evaluations for vertical and lateral homogeneity in terms of heteroatom distribution in the large-scale 2D TMD alloys are implemented. Se-stimulated strain effects and a detailed mechanism for the Se substitution in the MoS2 crystal are further explored. Finally, the capability of the 2D alloy for industrial application in nanophotonic devices and hydrogen evolution reaction (HER) catalysts is validated. Substantial enhancements in the optoelectronic and HER performances of the 2D ternary alloy compared with those of its binary counterparts, including pure-phase MoS2 and MoSe2 , are unambiguously achieved.

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