Department of Materials Science and Engineering Seminar Series 2025

Entropy-Driven Defect and Phase Engineering in Monolayer MoWSSe Alloys

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Date and time: 8th of December 2025 (Monday), 9:30 am to 11:30 am

Venue: S9, Level 9 Conference room

Abstract

Alloying in two-dimensional (2D) transition metal dichalcogenides (TMDs) enables access to structures and properties that are not attainable in binary crystals. Increased configurational entropy of alloys can be used to tune atom ordering, vacancy content, and defect density. This mechanism can be easily utilized in the synthesis of new materials for electro- and photocatalysis, optoelectronics, electronic and thermoelectric devices.

In this work, monolayer Mo-W-S-Se alloys are synthesized across a wide compositional range – from ternary lightly doped systems to quaternary equiatomic compositions – to investigate how configurational entropy can be used as an explicit design parameter. Increasing entropy through the incorporation of W and Se is shown to drive pronounced structural rearrangements, including trigonal prismatic (1H) to octahedral/distorted octahedral (1T/1T') phase transitions and the formation of a high density of chalcogen vacancies. Ternary MoSSe and $MoWS_2$ alloys exhibit spinodal decomposition, phase segregation, and strongly composition-dependent vacancy formation. In contrast, quaternary MoWSSe alloys form entropy-stabilized, vacancy-rich 1T lattices with higher structural and compositional uniformity. These alloys display markedly enhanced electrocatalytic activity for the hydrogen evolution reaction, with Tafel slopes and current densities approaching those of platinum, while maintaining stability under industrially relevant operating conditions.

Biography

Artemii S. Ivanov received his B.Sc. degree in Chemical Technology from St Petersburg Mining University in 2019 and his M.Sc. degree in Applied Chemistry from ITMO University in 2021. He is currently a Ph.D. candidate in the Department of Materials Science and Engineering at the National University of Singapore, under the supervision of Professor Konstantin S. Novoselov and Associate Professor Daria V. Andreeva-Baeumler. His research focuses on the synthesis and characterization of two-dimensional transition metal dichalcogenides, with an emphasis on defect and phase engineering for electro- and photocatalytic energy conversion.

Please join us!

HOST: Asst Prof Zhu Di