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Defect-induced ferroic states in solid solutions of layered van der Waals

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Solid solutions of transition-metal dichalcogenides (TMDs), a family of cuasi-2D van der Waals materials, provide a powerful platform to explore how composition, structural symmetry, and defect chemistry collectively determine electronic and ferroic properties in layered materials. In particular, the ability to independently tune substitutional disorder and intrinsic defect populations offers a route to stabilize emergent phases that are absent in stoichiometric compounds. These materials therefore offer a versatile framework to investigate how compositional engineering and defect-mediated symmetry breaking can generate new functional states.

In this talk, I will discuss how alloying different TMDs can be a general strategy to control structural symmetry and electronic instabilities that give rise to multiple ferroic orders. Within this framework, chemical substitution primarily modifies lattice parameters, bonding geometry, and spin–orbit coupling, while deviations from ideal stoichiometry introduce defect populations that can locally break inversion symmetry and generate magnetic moments or electric dipoles. The interplay between these two control parameters provides a pathway to stabilize magnetic, polar, and multiferroic states in otherwise non-ferroic layered materials.

I will illustrate these ideas with experimental examples from the alloy families WSe_2-WTe_2 and WS_2-WTe_2, synthesized as bulk single crystals and characterized through structural, magnetic, piezoresponse and transport measurements. In particular, the WSe_2-WTe_2 system reveals a systematic evolution of lattice symmetry and unit cell volume with tellurium substitution and the emergence of defect-stabilized magnetic and polar responses as the chalcogen vacancy density increases. By correlating substitution and defect concentration, a configurational ferroic phase diagram can be constructed that separates paramagnetic–ferromagnetic, paraelectric-ferroelectric, and multiferroic regimes. These results highlight how solid-solution engineering in layered van der Waals materials provides a general route to stabilize emergent ferroic phases through the coupled control of composition and defects.

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