Evidence of 2D Room-temperature Magnetic Semiconductors

Materials Discovery (In-house+Collaborators)

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Project Summary: Dilute magnetic semiconductors, achieved through substitutional doping of magnetic atoms into semiconducting systems, enable experimental modulation of spin dynamics for novel magneto-electric or magneto-optical devices, especially in 2D transition metal dichalcogenides that accentuate interactions and activate valley degrees of freedom. Practical applications of 2D magnetism will likely require room-temperature operation, air stability, and the ability to achieve optimal doping levels without dopant aggregation. 2DCC-MIP theorists collaborated closely with a highly interdisciplinary team of experimentalists both within and beyond the MIP to obtain evidence for room-temperature ferromagnetic order in vanadium-doped tungsten disulfide monolayers synthesized by a reliable single-step method with minimal dopant aggregation. First-principles calculations suggest that quenches due to orbital hybridization occurs at closer vanadium–vanadium spacings; this prediction is supported by transmission electron microscopy and magnetometry. These insights and discoveries help bring semiconducting 2D magnetic heterostructures closer to practical application.

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2DCC Role: First-principles theory of dopant energetics and mechanisms of magnetism, electron microscopy and collaborative synthesis.