Near room-temperature ferromagnetism and insulator-metal transition in van der Waals material $CrGeTe_3$

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Abstract:

We investigate the pressure-induced evolution of the electronic and magnetic properties of the van der Waals ferromagnet $CrGeTe_3$, a material that hosts ferromagnetism down to the monolayer and holds promise for near room-temperature applications. Using density functional theory (DFT) and dynamical mean-field theory (DMFT), we explore the transition from a low-temperature semiconducting ferromagnet to a near room-temperature metallic ferromagnet under pressure [1]. Complementing our theoretical analysis, experimental measurements of optical conductivity offer a detailed view of the evolution of electronic correlations, particularly through the insulator-to-metal transition. Crucially, we find that the optical gap persists in the metallic state, ruling out a simple collapse of the charge transfer gap under pressure and indicating more complex electronic interactions [2].

As pressure increases, a distinct mid-infrared (MIR) feature emerges in the optical conductivity, signaling the development of strong orbital-selective correlations in the high-pressure metallic phase [2]. We attribute these observations to orbital-specific electron and hole dynamics within the semi-metallic phase of $CrGeTe_3$. In combination, our experimental and theoretical results reveal that the double-exchange mechanism plays a key role in stabilizing near room-temperature ferromagnetism in $CrGeTe_3$.

Additionally, we explore the anomalous Hall effect (AHE) in $CrGeTe_3$ [3]. While our theoretical calculations predict a sign change in the anomalous Hall conductivity due to intrinsic Berry curvature effects, experimental observations show only an enhancement followed by a decay of the AHE under pressure. This leads us to conclude that the AHE is primarily driven by extrinsic mechanisms. We outline potential scenarios for these extrinsic contributions and their role in the AHE.

In summary, our findings demonstrate that near room-temperature ferromagnetism in $CrGeTe_3$ is driven by a double-exchange mechanism in the metallic phase. This suggests that both electron and hole doping can be utilized to achieve room-temperature ferromagnetism in $CrGeTe_3$. The material's tunable electronic and magnetic properties, along with its layered structure, make $CrGeTe_3$ a strong candidate for nanoscale magnetic devices.

References:

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