Electron correlation and complex magnetism in 2D Fe_nGeTe_2 (n=3-5) magnets

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Abstract
The Fe_nGeTe_2 (n=3, 4, 5) family of two-dimensional magnets has emerged as a potential candidate for spintronic applications. These magnets exhibit high temperature ferromagnetism, complex temperature dependent magnetization, structural reconstructions, skyrmionic features etc. Electron correlation, isotropic and anisotropic exchange interactions and magnetic anisotropy have enriched the overall magnetic properties, which require thorough investigations for a detailed understanding. Here, we present a systematic study of this family using first-principles electronic structure calculations with different flavors, viz. (i) standard density functional theory (DFT), (ii) static electron correlation (DFT+U) and (iii) dynamical electron correlation with dynamical mean field theory (DFT+DMFT). Moreover, complex structural aspects regarding site occupancy of Fe in Fe_5GeTe_2 [1] have been considered in connection to scanning tunnelling microscopy images. A thorough analysis of critical temperatures and spectral properties reveal [2] that DFT+DMFT is the most accurate method to correctly reproduce the experimental data on temperature dependent magnetization, valence band and angle-resolved photoemission spectroscopies respectively. Moreover, Monte Carlo simulations show peculiar magnetic structures at low temperature with site-selective canted Fe moments. The inaccurate values of structural parameters, magnetic moments and exchange interactions obtained from DFT+U make this method inapplicable for the FGT family. In summary, our study provides a comprehensive view of the electronic structure and magnetism of this important class of 2D magnets.

References

[1] S. Ershadrad, S. Ghosh, D. Wang, Y. Kvashnin and B. Sanyal, J. Phys. Chem. Lett. 13 (2022) 4877.
[2] S. Ghosh, S. Ershadrad, V. Borisov and B. Sanyal (submitted).