Emergent Superparamagnetism in TiS_2 Induced by Atomic-Scale Defects

Thomas M. Pekarek,[a] Patrick J. Keeney,[a] Kyle Taylor,[a] Cole Ratkus,[a] Jason T. Haraldsen[a] and Paula Mariel Coelho[a]

[a] *Department of Physics, University of North Florida, Jacksonville, FL 32224, USA*

Email: paulamariel.coelho@unf.edu

Defect engineering has emerged as a powerful route to induce and control magnetism in otherwise nonmagnetic two-dimensional materials [1]. Titanium disulfide (TiS_2), a layered transition metal dichalcogenide traditionally studied for energy storage and electronic applications, is nonmagnetic in its pristine form, making it an ideal platform to explore defect-driven magnetic behavior [2]. Here, we report the observation of superparamagnetism in bulk 1T-TiS_2 arising from clusters of intrinsic defects. In a comprehensive scanning tunneling microscopy (STM), superconducting quantum interference device (SQUID) magnetometry, and density functional theory (DFT) study, we identify Ti adatoms as the primary source of local magnetic moments [3]. SQUID measurements reveal a pronounced paramagnetic response, and a Brillouin fit yields an effective spin of 4. This surprisingly large magnetic response is consistent with cooperative clustering of Ti adatoms forming superparamagnetic centers. Atomically resolved STM images show a high surface concentration of point defects and well-defined triangular clusters, while DFT calculations confirm that both isolated Ti adatoms and small Ti clusters generate localized magnetic moments and enhanced collective magnetic responses. These results establish TiS_2 as a defect-tunable magnetic material, highlighting its potential for future application in spintronics.

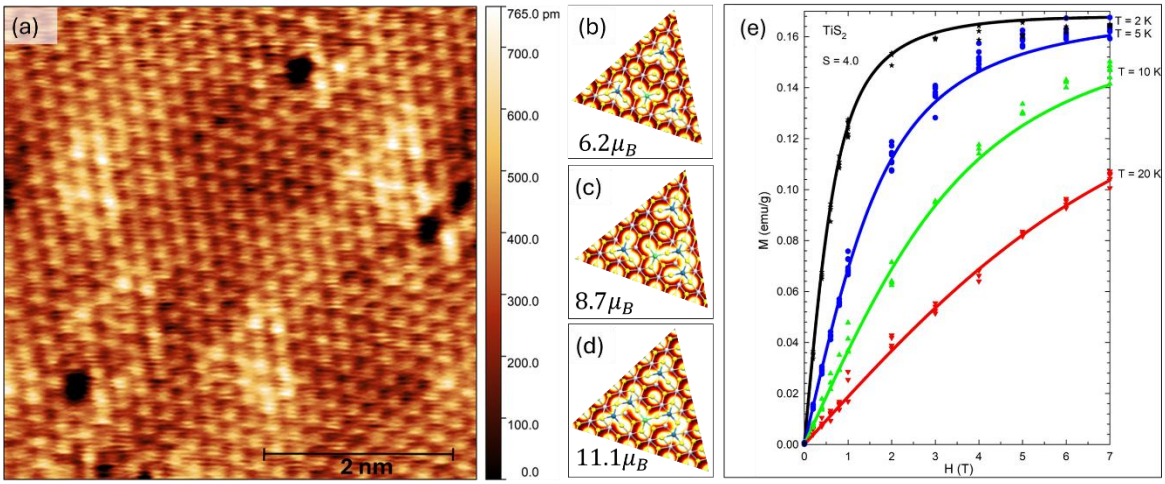

Figure 1: Comprehensive study on magnetic properties of defect clusters. (a) Atomically resolved STM topography images showing the formation of triangular cluster defects. Scanning parameters: V_B =0.3V and I_T = 0.3nA. (b)-(d): DFT calculations of potential configurations of Ti clusters, likely due to adatoms aligned to either a Ti atom (Ti_{top} in green) or a hollow site (H_{top} in blue) and their corresponding magnetic moments of clusters containing (b) 4, (c) 5, and (d) 6 titanium adatoms. (e) Magnetization versus applied field curves with Brillouin fits for 2, 5, 10, and 20 K for bulk 1T-TiS_2 yielding S = 4.0 as the best fit, a surprisingly high spin contribution.

[1] P.M. Coelho, J. Phys.: Condens. Matter **36** 203001 (2024)
[2] P. J. Keeney et al Nanomaterials **15**, 1435 (2025)
[3] T.M. Pekarek et al., under review (2026)