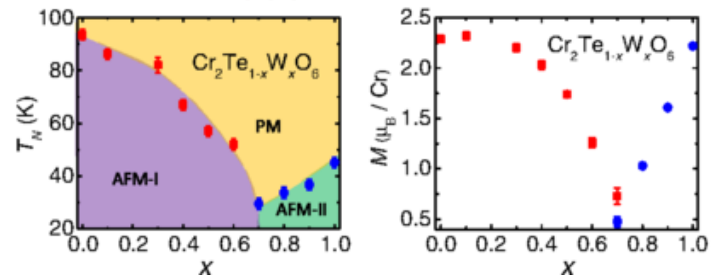
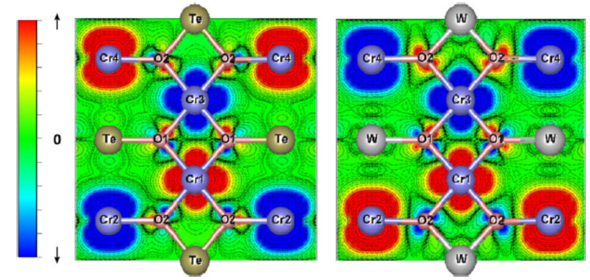
Neutrons Provide Insight into a New Approach to Tune Magnetic and Electronic Properties with Chemical Doping

Scientific Achievement

Neutron studies were used to reveal a complex magnetic phase diagram of $Cr_2(Te_{1-x}W_x)O_6$ systems. While compounds with different x values possess the same crystal structure, they display different magnetic structures below and above xc = 0.7, where both the transition temperature TN and sublattice magnetization (Ms) reach a minimum.



Left: TN–x phase diagram of $Cr_2(Te_{1-x}W_x)O_6$. PM represents the paramagnetic phase. Right: Magnetization as a function of x obtained from neutron powder diffraction measurements.



Spin densities (on (110) plane) of Cr2TeO6 (left) and Cr2WO6 (right) where red: spin up, blue: spin down.

Significance and Impact

This work introduces a new approach to tune the magnetic exchange via chemical doping: controlling the orbital hybridization between low energy unoccupied W 5d substituted into Te sites and O 2p states that provide the exchange path between two Cr moments.

Research Details

- The magnetic ground state of $Cr_2(Te_{1-x}W_x)O_6$ was determined by neutron powder diffraction.
- The spin density map was calculated using density functional theory (DFT) calculations.

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M. Zhu, D. Do, C. R. Dela Cruz, Z. Dun, H. D. Zhou, S. D. Mahanti, and X. Ke. *Phys. Rev. Lett*. 113 (2014): 076406.