Abstract Submitted
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Aspects of bulk and surface magnetism of magnetoelectric Fe_2TeO_6[1] SAI MU, KIRILL BELASHCHENKO, Department of Physics and Astronomy, University of Nebraska-Lincoln — Magnetoelectric antiferromagnets can be used to implement voltage-controlled magnetism, but materials design for above room-temperature operation is a challenge. Here we focus on the trirutile Fe_2TeO_6 magnetoelectric and use first-principles calculations to develop several strategies for increasing its Néel temperature T_N above the bulk 210 K value. We find that substitution of larger ions like Zr or Hf for Te increases T_N by increasing the superexchange angles. The compensating O vacancies tend to form bound complexes with such dopants, preserving the electronic band gap. Substitution of N for O is favorable due to the decreased charge-transfer gap. T_N is also increased by compressive [001] epitaxial strain. To help interpret the XMCD signal observed from the (110) surface of Fe_2TeO_6,[2] we compare the energies of several terminations of this surface and find the known TiO_2-like termination is the most stable. The perpendicular magnetic moment at this surface, which appears through spin canting due to spin-orbit coupling, is found to be only 0.015 μ_B per surface Fe. The XMCD signal likely originates from the lowered symmetry of the combined surface and X-ray beam configuration.

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[2]Wang *et al.*, J. Phys: Condens. Matter 26, 055012 (2014)

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