Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Itinerant antiferromagnetism in RuO_2[1] PAUL SNIJDERS, TOM BERLIJN, Oak Ridge National Laboratory, OLIVIER DELAIRE, Duke University, HAIDONG ZHOU, University of Tennessee, THOMAS MAIER, HUIBO CAO, SONGXUE CHI, MASAAKI MATSUDA, YANG WANG, Oak Ridge National Laboratory, MICHAEL KOEHLER, University of Tennessee, PAUL KENT, Oak Ridge National Laboratory, HANNO WEITERING, University of Tennessee — Bulk rutile RuO_2 has long been considered a Pauli paramagnet. Here we report that RuO_2 exhibits a hitherto undetected lattice distortion below approximately 900 K. The distortion is accompanied by antiferromagnetic order up to at least 300 K with a small room temperature magnetic moment of approximately 0.05 B as evidenced by polarized neutron diffraction. Density functional theory plus U (DFT+U) calculations indicate that antiferromagnetism is favored even for small values of the Hubbard U of the order of 1 eV. The antiferromagnetism may be traced to a Fermi surface instability, lifting the band degeneracy imposed by the rutile crystal field. The combination of high Néel temperature and small itinerant moments make RuO_2 unique among ruthenate compounds and among oxide materials in general.

[1]This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

Paul Snijders
Oak Ridge National Laboratory

Date submitted: 10 Nov 2016 Electronic form version 1.4