MAR16-2015-004353

Abstract for an Invited Paper for the MAR16 Meeting of the American Physical Society

High antiferromagnetic transition temperature for a layered hexagonal compound: $SrRu_2O_6^1$ JIAQIANG YAN, Oak Ridge National Laboratory and University of Tennessee

4d or 5d transition metal oxides (TMOs) are less correlated and have a larger bandwidth than 3d TMOs. A high magnetic ordering temperature for 4d/5d TMOs is not expected. It was therefore a surprise when a perovskite, $SrTcO_3$, was reported to order magnetically around 1000 K. Unfortunately, the radioactive nature of Tc prevented further investigation of the underlying mechanism for the high magnetic ordering temperature. Here we report antiferromagnetic order of $SrRu_2O_6$ at 565 K. Two features distinguish this compound from $SrTcO_3$: (1) $SrRu_2O_6$ is not radioactive, which allows the study of the underlying physics by a large variety of techniques as well as the possible fine tuning of the magnetic ground state; and (2) $SrRu_2O_6$ crystallizes into a quasi-two-dimensional structure with layers of edge-sharing RuO_6 octahedra separated by nonmagnetic Sr layers. Our density functional calculations and Monte Carlo simulations suggest an origin of the reduced moment size and the high Neel temperature.

¹Work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division and by the CEM and NSF MRSEC under Grant No. DMR-1420451.