## Abstract Submitted for the MAR13 Meeting of The American Physical Society

Magnetic properties and electronic structure of  $Cr_2(Te_{1-x}W_x)O_6^{-1}$ X. KE, D. DO, Department of Physics and Astronomy, Michigan State University, H. ZHOU, Department of Physics and Astronomy, University of Tennessee, C.R. DELA CRUZ, Quantum Condensed Matter Division, Oak Ridge National Laboratory, S.D. MAHANTI, M. ZHU, Department of Physics and Astronomy, Michigan State University — We report magnetic properties of  $Cr_2(Te_{1-x}W_x)O_6$  system combining neutron powder diffraction measurements and first principles electronic structure calculations. Both the end members possess an ordered inverse-trirutile structure, in which there are bilayers of Cr-O separated by a W(Te)-O layer, yet  $Cr_2TeO_6$ and  $Cr_2WO_6$  display distinct magnetic structures and antiferromagnetic transition temperatures:  $T_{\rm N} \sim 92$  K for  $Cr_2 TeO_6$  with antiferromagnetic spin alignment within bilayers, while  $T_{\rm N} \sim 45$  K for  $\rm Cr_2 WO_6$  with spins aligned ferromagnetically within the bilayer. Spins belonging to neighboring bilayers are antiferromagnetically coupled for both the compounds. For the mixed system  $Cr_2(Te_{1-x}W_x)O_6$ , both  $T_N$  and sublattice magnetization  $(M_{\rm s})$  reach a minimum  $(T_{\rm N} \sim 0 \text{ K})$  for  $x \sim 0.6$ , suggesting the existence of a quantum critical point. Electronic structure calculations using abinitio density functional theory correctly give the ground state spin configurations for the end compounds (x=0,1). We suggest that unoccupied W 5d states play a key role in intra-bilayer ferromagnetic ordering seen in the x=1 system.

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