Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Giant spin-phonon coupling in a 5d NaOsO3[1] STUART CALDER, JUN HEE LEE, MATHEW STONE, MARK LUMSDEN, Oak Ridge National Lab, JONATHAN LANG, APS, MIKHAIL FEYGENSON, Oak Ridge National Lab, YOUGUO SHI, CAS, YING SUN, YOSHIHIRO TSUGIMOTO, KAZUNARI YAMAURA, NIMS, ANDREW CHRISTIANSON, Oak Ridge National Lab — The coupling of distinct properties offers avenues to multifunctional materials. A limiting factor, however, is the degree that one parameter has to be modified to sufficiently alter the coupled property. Through a neutron scattering and first-principles density functional theory study of the 5d perovskite $NaOsO_3$ we reveal that from only a 0.1% lattice change an unprecedentedly large coupling emerges. The manifestation is a "giant" spin-phonon coupled mode shift of $\Delta\omega$=40 cm^{-1}, the largest observed in any material. By identifying the dominant phonon as the octahedral breathing mode we show isosymmetric ordering and cooperation between the lattice and the exotic magnetically driven Slater metal-insulator transition in this material. The occurrence of the dramatic spin-phonon-electronic coupling in $NaOsO_3$ is due to a property common to all 5d materials: the large spatial extent of the 5d ion. Consequently examining 5d materials in a new light offers novel routes for multifunctional devices with enhanced coupled phenomena.

[1]A portion of this research at ORNL's High Flux Isotope Reactor and Spallation Neutron Source was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

Stuart Calder
Oak Ridge National Lab

Date submitted: 14 Nov 2014 Electronic form version 1.4