

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Local orbital fluctuations and $t2g$ degeneracy lifting in the metallic regime of CuIr_2S_4 ¹ EMIL S. BOZIN, MILINDA ABEYKOON, Brookhaven National Lab, ALEXANDROS LAPPAS, IESL FORTH, YEW SAN HOR, JOHN F. MITCHELL, Argonne National Lab, SIMON J.L. BILLINGE, Brookhaven National Lab — High temperature metallic regime of CuIr_2S_4 possessing $\text{Fd}\bar{3}m$ cubic average structure is found to exhibit local structural distortions of the pyrochlore Ir sublattice compatible with tetragonal $I4_1/amd$ structure. X-ray total scattering based atomic pair distribution function approach further shows that the distortions are stabilized by Cr-doping induced strain fields, but remain poorly spatially correlated. Presence of such local spatially (and presumably temporally) fluctuating tetragonal distortions suggests that the $t2g$ orbital degeneracy is already lifted locally deep in the metallic regime (such a state persists up to at least 780 K), as a precursor to the metal-insulator transition (MIT) which is observed at low temperature (230 K). Underlying short range orbital ordering is limited to the nearest neighbor Ir-sites only, resembling orbital liquid-like state. This observation provides a rationale for reportedly poor and unusual metallicity at high temperature, and further suggests that the MIT can be seen, at least in part, as crystallization into a long-range orbitally ordered lattice. Notably, Ir-dimer order seen in the insulating phase melts across the MIT on all length-scales, and no dimers survive in the metallic state, as reported earlier.

¹Work at BNL was supported by US DOE-BES under Contract DE-SC0012704. Work at ANL was supported by DOE-BES, MSE Division. AL acknowledges support from the Fulbright Foundation.

Emil Bozin
Brookhaven National Lab

Date submitted: 07 Nov 2016

Electronic form version 1.4