Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Correlations in lacunar spinels: dynamical mean-field study with configuration interaction based impurity solver[1] ARA GO, Department of Physics, Columbia University, HEUNG-SIK KIM, Department of Physics, University of Toronto, HOSUB JIN, Center for Correlated Electron Systems, Institute for Basic Science / Department of Physics and Astronomy, Seoul National University, ANDREW MILLIS, Department of Physics, Columbia University — Density functional plus dynamical mean field methods are used to study the role of correlations in in lacunar spinel compounds GaM_4X_8 (M=Nb, Mo, Ta and and X=S, Se and Te) to investigate the interplay of correlations and topology in materials with strong spin-orbit coupling. A novel configuration-interaction exact diagonalization solver enables inclusion of more bath orbitals, enabling a better treatment of spectral functions and more accurate computations of phase boundaries. Focussing on $GaTa_4Se_8$, we discuss how the correlation induces metal-insulator transition in presence of the spin-orbit coupling, based on spectral functions and optical conductivities.

[1]This work was supported by the US Department of Energy under Grants No. DOEFG02-04ER46169 and DE-SC0006613.

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Date submitted: 13 Nov 2014 Electronic form version 1.4