Towards New and Higher Temperature Superconductors via Theory Assisted Synthesis\textsuperscript{1}

MEIGAN ARONSON, Stony Brook University and Brookhaven National Laboratory

We discuss here a new methodology where electronic structure calculations are integrated with the synthesis of new superconducting materials, with the objective to design and realize new lamellar superconductors with high onset temperatures, and to rigorously test the apparent association of high temperature superconductivity with electron delocalization transitions occurring at quantum critical points. Since lamellar superconductors like the cuprates and iron pnictides are comprised of functional layers where superconductivity resides and charge reservoir layers that determine the electron count in the functional layers, we will use realistic electronic structure calculations to assess which transition metal monopnictides are closest to electron delocalization, and hence optimal for superconductivity. Optical conductivity and photoemission measurements will be used to compare the real and calculated electronic structures. We report initial results on electron and hole doped LaMnPO.

\textsuperscript{1}This research is carried out in collaboration with G. Kotliar, D. Basov, and H. Tjeng under the auspices of an NSSEFF fellowship administered by the AFOSR.