MAR16-2015-002253

Abstract for an Invited Paper
for the MAR16 Meeting of
the American Physical Society

Towards the design of novel cuprate-based superconductors

CHUCK-HOU YEE, Rutgers Univ

The rapid maturation of materials databases combined with recent development of theories seeking to quantitatively link chemical properties to superconductivity in the cuprates provide the context to design novel superconductors. In this talk, we describe a framework designed to search for new superconductors, which combines chemical rules-of-thumb, insights of transition temperatures from dynamical mean-field theory, first-principles electronic structure tools, materials databases and structure prediction via evolutionary algorithms. We apply the framework to design a family of copper oxysulfides and evaluate the prospects of superconductivity.