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In situ measurements of high temperature growth of correlated systems: a materials by design scheme¹
HUA HE², Department of Physics Astronomy, Texas A M University

There is great interest in developing new ways to use predictive theory to accelerate materials synthesis. We have previously shown that DFT+DMFT electronic structure calculations are successful at predicting gaps and ordered moments, even when correlations are very strong.^[1,2] Building on these results, we set out to explore an even closer integration of theory and synthesis, aiming to discover new routes for doping Mott insulators and producing new superconductors. In situ high temperature high energy X-ray diffraction is used to determine the crystal structures of compounds just as they form from the growths, and the structural information is used as input for DFT+DMFT calculations that predict functionality, closing the synthesis loop by suggesting productive new directions. Using this approach, we have investigated the transition metal oxysulfide system Ba-Co-S-O and successfully discovered the new compound BaCoSO, and identified it as an interesting small gap Mott insulator by DFT+DMFT calculations even before any traditional crystal growth is attempted in the lab. [1] J. W. Simonson, et al. Proc. Nat. Acad. Sci. 109 (2012) E1815 [2] J. Guo, et al. Nat. Sci. Rep. 3 (2013) 2555

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