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The Iron Age of Superconductivity: Chemistry and Physics based on Electronic Structure Studies

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2:30 P.M.

210 Robeson

The 2008 discovery of high temperature superconductivity in doped LaFeAsO by Kamihara and co-workers provided the second class of high Tc materials, the other being the cuprate family discovered in 1986 by Bednorz and Mueller. This discovery was revolutionary in that many of the properties of the iron based superconductors are radically different from those of the cuprates, apparently requiring a new and broader understanding of the physics of high temperature superconductivity. The purpose of this talk is to discuss the chemistry and physics of the new superconductors in relation to cuprates. So far, many puzzles remain. The materials appear to be much more band-like and show much stronger signatures of metallic (Fermi surface related) physics than cuprates, with correspondingly weaker signatures of on-site Hubbard correlations. However, there remain substantial discrepancies between bare band structure calculations and experiment, and interestingly these discrepancies are in the opposite direction from those found in cuprates. These are discussed in the context of spin-fluctuations. A remarkable feature of the iron based materials is that superconductivity can be induced by alloying on the iron site both in LaFeAsO type and in ThCr2Si2 structure materials. The chemistry of these alloys is discussed in terms of their bonding as revealed by electronic structure calculations and experiment. Finally, the possible superconducting pairing is discussed in terms of spin fluctuations based on the electronic structure, and some of the many open questions are laid out.