Structural Distortions under pressure and doping in superconducting BaFe$_2$As$_2$

SIMON KIMBER, Helmholtz Zentrum Berlin

The discovery of a new family of high-$T_C$ materials, the iron arsenides, has led to a resurgence of interest in superconductivity. Several important traits of these materials are now apparent: for example, layers of iron tetrahedrally coordinated by arsenic are crucial structural ingredients. The structure and properties of chemically substituted samples are known to be intimately linked; however, until recently (1), remarkably little was known about this relationship when high pressure is used to induce superconductivity in undoped compounds. Here we show that the key structural features in BaFe$_2$As$_2$ show the same behaviour under pressure as found in chemically substituted samples. Using experimentally derived structural data, we show that the electronic structure evolves similarly in both cases. Our results show that, in contrast to the cuprates, structural distortions are more important than charge doping in the iron arsenides. This work was performed at the Helmholtz-Zentrum Berlin in collaboration with Ames Laboratory, Goethe-Universität Frankfurt, JCNS Jülich and the Institute Laue-Langevin. (1) S.A.J. Kimber et al, Nature Materials,