Electronic structure of iron-pnictide superconductors: just scratching the surface.

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Angle resolved photoemission (ARPES) and scanning tunneling microscopy (STM) give complimentary, real and momentum space pictures of the electronic structure of solids. They are widely used in the study of correlated electronic systems, for instance in the study of iron-pnictide high temperature superconductors. These techniques are however surface sensitive and one has to ensure that the electronic structure probed in an experiment corresponds to the bulk electronic structure. This turns out to be particularly important for the iron-pnictides that are layered structures with alternately charged layers. The surface of such a system is unstable and is usually reconstructed in some way.

Using a combination of experimental techniques (STM, ARPES, LEED) and theoretical calculations (LEED simulations, DFT), I will show that the surface is indeed reconstructed in the most widely studied iron-pnictide superconductor, BaFe$_{2-x}$Co$_x$As$_2$. As a first step, the LEED data combined with simulations is used to solve the real surface and sub-surface structure. The impact of the surface on the electronic structure can then be determined by comparing DFT slab calculations, based on the real surface structure, with ARPES experiments. I will show that the presence of surface states gives a natural explanation for the large k-space broadening observed in these materials. Having identified the surface states and bulk bands, we are now in a position to address the more important questions with regard to the electronic structure and its role in the mechanism of high temperature superconductivity.

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