A first-principles description of stronger correlations: topological phases to stripes in cupates

Arun Bansil

Physics Department, Northeastern University, Boston, Massachusetts

I will discuss how advanced density functionals are enabling new insights into the electronic structures, phase diagrams, and magnetism of topological materials, novel superconductors, atomically thin 2D films, among other materials. Illustrative examples drawn from our recent work will include [1-7]: (i) How by exploiting electronic structure techniques we have been able to successfully predict and understand the characteristics of many new classes of topologically interesting materials, including magnetic topological materials; (ii) How atomically thin beyond-graphene 2D and layered materials offer exciting new possibilities for manipulating electronic structures and topology and provide novel platforms for fundamental science studies and applications; And, (iii) regarding the high-T_c superconductors, I will discuss recent breakthroughs in modeling the insulating pristine compounds and their transition from the insulating to the metallic state with doping without invoking free parameters such as the Hubbard U parameter. A first-principles description of the competing stripe and magnetic phases in the cuprates also then becomes possible, providing a new pathway for modeling correlated materials more generally, despite the inability of the theory to capture some salient features of the correlated spectrum.

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[7] A. Bansil, H. Lin and T. Das, *Reviews of Modern Physics* 88, 021004 (2016).