Electronic Structure and Modeling of Highly Resolved Spectroscopies in Topological Insulators and Other Complex Materials

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We have been developing and implementing methodologies for unfolding how electronic structure of a complex material is reflected in various highly resolved spectroscopies such as angle-resolved photoemission (ARPES), scanning tunneling microscopy (STM) and inelastic x-ray or neutron scattering. Motivation is that spectroscopies do not provide a direct map of the electronic spectrum, but act as a very complex 'filter' or 'mapping' of the energy levels, Fermi surfaces and excitation spectra of interest. We may refer to this link between theory and experiment as a generalized 'matrix element' effect, which differs greatly between different spectroscopies. Realistic modeling of the matrix element effects is of key importance not only for a robust identification of the origin of specific spectral features, but also for designing discriminating tests of competing theoretical models, and as a rational basis for further experimentation and model building. In this context, I will comment first on our work on topological insulators, which has so far has been focused mainly on predicting new topologically interesting binary, ternary and quaternary material classes using more or less standard electronic structure techniques.[1-4] This will form a natural basis for discussing our ongoing effort aimed at modeling realistically ARPES and STM spectra from topological surface states and the associated spin-textures via first-principles methods as well as by deploying appropriate tight-binding model Hamiltonians informed as far as possible by first-principles band structures. Finally, I will comment on a comprehensive, beyond LDA scheme we have been developing for addressing various spectroscopies where effects of matrix elements are accounted for in the presence of strong electronic correlations, superconductivity and pseudogap physics. A few illustrative examples drawn from our recent studies where surprising insights into the nature of electronic structure and correlation effects in the cuprates and other complex materials have been obtained through spectroscopic modeling will be presented. [5-8]

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