Recent Progress in Modeling Electronic Structure and Spectroscopy of Topological Insulators and Novel Superconductors

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I will discuss some of our recent results aimed at understanding the electronic structure and spectroscopy of novel superconductors, topological materials, and atomically thin 2D films. [1-9] Illustrative examples include: (i) How by exploiting electronic structure techniques we have been able to predict and understand the characteristics of many new classes of binary, ternary and quaternary topologically interesting materials, inclduing topological crystalline insulators; (ii) How atomically thin 'beyond graphene' 2D materials such as silicene, germanene, stanene, and $MoSe_2$ offer exciting new possibilities for manipulating electronic structures and the associated topological phases, providing novel platforms for various applications; (iii) Asymmetry of the scanning tunneling (STM) spectrum of the cuprate high-Tc superconductors between positive and negative bias voltages and the extent to which it comes about within the conventional picture, and how strong correlation effects modify the STM spectra; (iv) The character of the doped holes in the curpate superconductor La-Sr-Cu-O as revealed by the analysis of doping dependent high-resolution Compton scattering studies.

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