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First-principles Wannier function based methods for disordered materials and applications to studies of oxides and Fe-superconductors[1]

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This talk will discuss recently developed first-principles methods for materials with disordered impurities, and their applications to case studies of correlated oxides and Fe-based superconductors containing vacancies, substitutions and intercallants. Simplified via the use of Wannier functions, the first method [1] is to unfold the one-particle spectral function from the reduced Brillouin zone of a broken symmetry state back to the regular Brillouin zone of the normal state. This unfolding not only allows a clearer visualization of the physical effects of the broken translational symmetry, but also connects directly to the experimental spectral weight of angular resolved photo emission spectroscopy. The second method [2] is to reduce the computational expense of configuration-averaged spectral function of disordered materials by orders of magnitude, to allow inclusion of large length scale required for weakly localized states and short-range orders. This Wannier function based method is systematically improvable, beyond-mean-field, and not perturbation limited. Case studies to be discussed include dilute magnetic semiconductors [3], transition metal oxides[1,2], and Fe-based superconductors [4,5].

[1] Wei Ku et al, PRL 104, 216401 (2010)
[2] T. Berlijn et al, PRL 106, 077005 (2011)
[3] T. S. Herng et al, PRL 105, 207201 (2010)
[4] C.-C. Lee et al, PRL 103, 267001 (2009)
[5] C.-H. Lin et al, arXiv:1107.1485

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