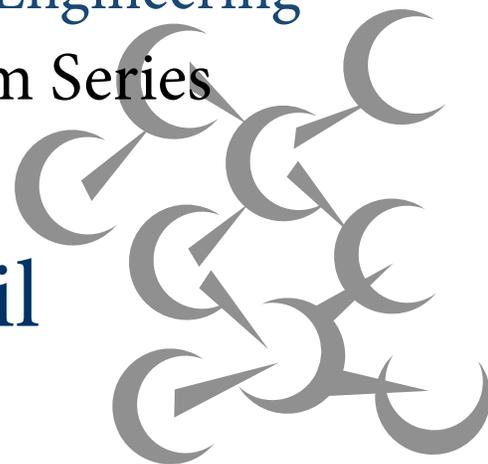


# Chemical & Environmental Engineering 2009 - 2010 Colloquium Series



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### Modeling Highly Resolved Spectroscopies of Complex Materials: From Qualitative to Quantitative

We stand at the threshold of a new 'golden age' of spectroscopic studies of materials for unraveling how charge, spin, orbital and lattice degrees of freedom interact to produce emergent phenomena and exotic states of matter. In this connection, the need for realistic modeling of various highly resolved spectroscopies is becoming of critical importance in providing discriminating tests of competing theoretical models and as a rational basis for future experimentation. In this talk, I will discuss how as we move to model spectroscopic data from a qualitative to a quantitative level, surprising new insights into the nature of electronic states and correlation effects are obtained in high-temperature cuprate superconductors and other complex materials.[1-6] Illustrative examples in cuprates include: (i) Asymmetry of the scanning tunneling (STM) spectrum between positive and negative bias voltages and the extent to which it comes about within the conventional picture; (ii) Origin of the 'high-energy kink' or the 'waterfall effect' in the photoemission spectrum (ARPES) and the interplay therein between effects of the matrix element and the presence of strong coupling of the quasiparticles to electronic excitations; and (iii) The nature of the dichroic signal in photoemission and its relationship to the time-reversal symmetry breaking in the cuprates. I will also comment on our recent work on the manganites and topological insulators.

Friday December 4, 2009

9:30 - 10:30 AM

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