

# Physics Seminar

## Michigan Technological University

Monday, July 14, 2008  
11:00 am  
Room 130, Fisher Hall

### Multi-reference Coupled-cluster Approach for Spectra and Properties Sourav Pal

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#### Abstract

Development and application of Fock space multi-reference coupled-cluster (FSMRCC) method for high performance electronic structure, spectra and properties will be highlighted. We will present our recent formulation of analytic response of FSMRCC, which has facilitated the efficient computation of analytic energy derivatives using FSMRCC method. In particular, our applications to molecular electric properties will be highlighted. Recent computation of electronic excitation energies of model quantum dots using FSMRCC method as well as resonance and width of electron-molecule resonance will also be presented.