Time-Dependent Density Functional Theory: Ground State, Excited State, and Beyond . . .

Monday, April 27, 2009

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3:30 p.m. Room 8335

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In this talk, I will present our recent developments of TDDFT, including a multi-reference linear response theory for modeling multiple-electron excited state, and the real-time non-perturbative TDDFT method. These new TDDFT developments will be integrated with applications for studies of diluted magnetic semiconductor nanocrystals, lifetimes of excited states, and intense laser controlled molecular reactions.

Theoretical Chemistry Institute Seminar Series