



Monday, October 14, 2019, 12:00 pm
Zumberge Hall of Science, ZHS 159

Professor Eric Neuscamman

*Department of Chemistry
University of California Berkeley*

Excited-State-Specific Quantum Chemistry

Theoretical models for excited states play crucial roles throughout chemistry and materials science, from understanding light harvesting and photo-catalytic mechanisms to the design and interpretation of spectra. However, methods for modeling excited states and their properties are at a fundamental disadvantage when compared to ground state methods, as they rely on additional layers of approximation beyond what ground state theories require. One can see this pattern play out across electronic structure theory, from the adiabatic approximation in time-dependent density functional theory to the assumption that all states have the same orbitals in state-averaged multi-reference theory. In contexts such as charge transfer and multiply excited states, these approximations limit the accuracy and predictive power of current methodology.

Very recently, it has become clear that excited state variational principles can be used to reformulate excited state methods so that they no longer require additional approximations beyond those used for ground states. I will discuss how these variational principles allow essentially the whole range of ground state methodology, from Hartree Fock and density functional theory to perturbation theory, coupled cluster theory, multi-reference theory, and even quantum Monte Carlo to be rebuilt in a framework that is wholly excited-state specific.

Suggested Reading:

1. Flores, S. D. P.; Neuscamman, E. Excited State Specific Multi-Slater Jastrow Wave Functions. *The Journal of Physical Chemistry A*. **2019**, 123 (8), 1487–1497. <https://doi.org/10.1021/acs.jpca.8b10671>
2. Shea, J. A. R.; Neuscamman, E. Communication: A Mean Field Platform for Excited State Quantum Chemistry. *The Journal of Chemical Physics* **2018**, 149 (8), 081101. <https://doi.org/10.1063/1.5045056>

Hosted by Professor Anna Krylov

The scientific community is invited

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