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CHEMISTRY SEMINAR 291

Variational Principles for Excited States

Date: **2/9/18**
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Location: **COB1 267**

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ABSTRACT

The ground state variational principle is perhaps the single most important theoretical tool in quantum chemistry, directly or indirectly supporting everything from density functional theory to coupled cluster theory. It's ability to tailor every aspect of a wave function for a specific electronic state (the ground state) maximizes the accuracy that can be wrought from simple wave function approximations. Historically, this advantage has been exclusively available to the ground state, with excited states modeled by other methods like linear response that are much less capable of tailoring the details of a wave function, such as its orbital shapes, for an individual excited state. We will discuss recent progress in overcoming the challenges that have long inhibited the development and use of rigorous excited state variational principles that promise to level the playing field, as well as the areas of chemistry (charge transfer complexes and x-ray spectroscopy are two) that are likely to be the most strongly impacted by these advances.

BIO:

Professor Neuscamman mostly grew up in CA, and was an undergrad at UCLA. He then did his PhD at Cornell with Garnet Chan, and a postdoc at Berkeley as a Miller Fellow, followed by a postdoc at LLNL as a Lawrence Fellow. He has been an Assistant Professor at UC Berkeley since summer 2015.