



**CHEMISTRY &
BIOCHEMISTRY**

DATE 11/14/2025 | **TIME** 01:30pm | **LOCATION** COB1 267

CHEMISTRY & BIOCHEMISTRY SEMINAR SERIES: Ensemble Time Dependent Density Functional Theory

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Abstract:

Linear Response Time-Dependent Density Functional Theory (LRTDDFT) gives access to accurate transition frequencies and oscillator strengths of low-lying optical excitations. However, because LRTDDFT is based on small perturbations around the ground-state potential, it cannot describe transitions between excited states, crucial to explain, for example, pump-probe laser experiments. Recently, an alternative approach to obtain transition frequencies—Ensemble DFT—has regained attention, which incorporates information about all eigenstates in its ensemble. By combining these methods, Ensemble TDDFT (ETDDFT) offers a variety of new cost-effective approaches to recover excited-state to excited-state transitions and double excitations that are beyond LRTDDFT's reach. In this talk, we present exact ensemble formulations of key equations, such as the Adiabatic Connection Fluctuation-Dissipation Theorem. These exact and approximate results are illustrated using the symmetric two-site Hubbard model at half-filling.

About the Speaker:

Kimberly Daas is working in the field of theoretical chemistry, which is on the intersection between chemistry, physics, mathematics and even computer science. Her research interests are increasing our current understanding of electronic structure theory and in particular Density Functional Theory, the workhorse of quantum chemistry, and deriving new practical approximations for it. She received her bachelor's and master's degrees as a Joint Degree at both the Universiteit van Amsterdam (UvA) and the Vrije Universiteit Amsterdam (VU), respectively in Chemistry (2017) and Molecular Sciences (2019). The research for both theses was done in the group of Prof. Dr. Gori-Giorgi at the VU, which is also the group she did her PhD research in. In her dissertation, The Strong Interaction Limit of The Moller- Plesset Adiabatic Connection, she not only derived a new exact theory but also provided accurate practical approximations for it. Using these results, she derived new functionals that can be used in both chemistry and material science to calculate non-covalent interactions, which are generally weak interaction that play important roles in (bio)-chemistry by keeping our DNA double helices together and enabling enzymatic reactions. She is currently an UCI's Chancellors Postdoctoral Fellow in the group of Prof. Dr. Burke, where here focus has been on deriving the exact theory of Ensemble Time Dependent Density Functional Theory and making a new Machine Learned DFT functional that is specifically build for materials.

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