# VISTA Seminar

## Seminar 74

**September 4, 2024**

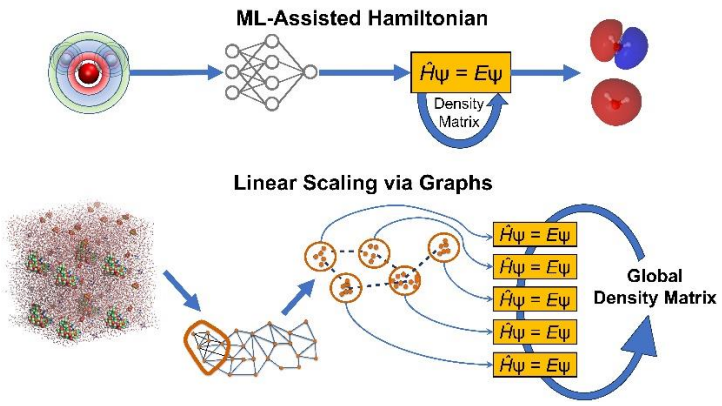
**10:00 am – 11:30 am EDT / 3:00 – 4:30 pm BST London / 4:00 pm – 5:30 pm CEST Paris / 10 pm – 11:30 pm CST Beijing**

**TOC:**

# Advancing Quantum Simulations with Machine Learning and Graph Theory

Maksim Kulichenko

*Los Alamos National Laboratory, T-1 (Physics and Chemistry of Materials), Los Alamos, NM, USA. Email: maxim@lanl.gov*

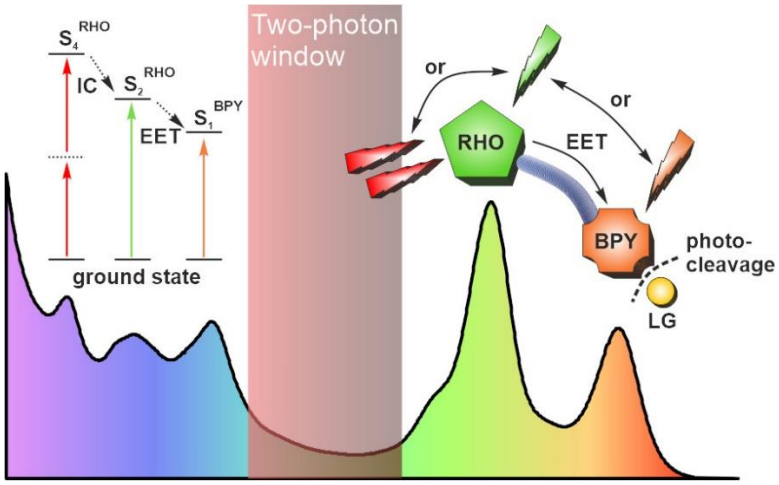



Machine learning is rapidly transforming the landscape of quantum simulations, offering new possibilities for modeling dynamical processes at atomic resolution. Modern ML models go beyond near-equilibrium ground state simulations and can deal with complex reactive events and excited state dynamics. In my talk, I will present recent advancements made at the Theoretical Division, LANL, in the area of ML-assisted quantum simulations. First, I will discuss the application of machine learning potentials to dynamical and reactive simulations. Next, I will address the limitations of purely ML-based models and discuss strategies to enhance their performance by integrating them with approximate quantum models. Finally, I will showcase our latest findings in graph-based quantum dynamics, a promising approach that achieves nearly linear scaling, enabling quantum simulations of extremely large systems.

# Decoherence in molecular systems with structured spectral densities studied with Gaussian wavepacket propagation

Sreeja Loho Choudhury

*Institute of Physical and Theoretical Chemistry, Goethe University Frankfurt, Germany*
*Email: dreamysreeja@gmail.com*




We investigate the time scale of decoherence in complex molecular systems following laser excitation [1]. Vibronic coupling Hamiltonians in conjunction with realistic, structured spectral densities are employed in order to track decoherence on a typical time scale of femtoseconds. Tensor network methods, notably the Gaussian-based Multi-Configuration Time-Dependent Hartree approach [2], are used to obtain accurate decoherence estimates obtained from the time-evolving purity. Finite temperature is included via the thermofield dynamics approach. We focus on a donor-acceptor system that has recently been studied [1], comprising tens of vibrational degrees of freedom. This system is subject to a coherent excitation energy transfer (EET) process and exhibits irreversible decay features despite the finite dimensionality. Numerical decoherence decay is compared with analytical estimates for pure dephasing in spin-boson systems [3-5]. The transition between Gaussian vs. exponential purity decay is discussed.

**References:**

[1] M. Asido et al., Phys. Chem. Chem. Phys. 24, 1795 (2022).
[2] P. Eisenbrandt, M. Ruckenbauer and I. Burghardt, J. Chem. Phys. 149, 174102 (2018).
[3] O. Prezhdo and P. Rossky, Phys. Rev. Lett. 81, 5294 (1998).
[4] B. Guo and I. Franco, J. Phys. Chem. Lett. 8, 4289 (2017).
[5] M. A. Schlosshauer, Decoherence and the Quantum-To-Classical Transition, Springer (2007).

# How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 74
Time: Sep 4, 2024 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting
https://buffalo.zoom.us/j/92788064450?pwd=EuCyDpJvJ0uo5EYnqYa2tUhO9dAGQU.1

Meeting ID: 927 8806 4450
Passcode: 831918