PHYSICS COLLOQUIUM:
Molecules in Quantum Motion

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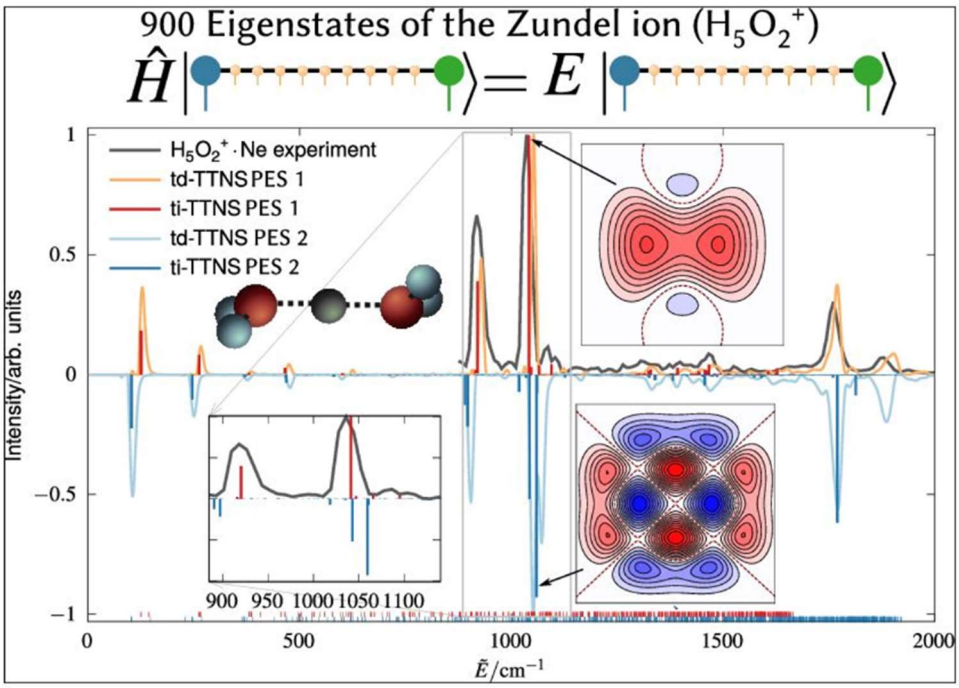
Date:
10/21/2022

Time:
10:30 AM-11:50 AM

Location:
KOLLIG 217

Abstract:

In order to fully understand the nature of molecules, we need to simulate both the electronic and vibrational motion quantum mechanically. However, simulations of quantum many-body systems, such as molecules, scale exponentially with system size. I will explain how to tame this 'curse of dimensionality' by combining methods from the traditionally disjoint fields of electronic structure, condensed matter physics and nuclear dynamics, in particular the density matrix renormalization group (DMRG) and related tensor network states. This combination has enabled the simulation of complex systems with unprecedented accuracy and speed. I will demonstrate how these methods make it possible to solve a diverse set of problems, ranging from characterizing hydrated protons on a molecular quantum level to the accurate computation of ground state potential energies of strongly correlated metal clusters. I will demonstrate how these simulations provide new insights into complex experimental results.



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