UCLA College | Physical Sciences Chemistry & Biochemistry

THEORETICAL PHYSICAL CHEMISTRY SEMINAR

Dr. Henrik Larsson

Postdoctoral Scholar
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Tuesday, Jan. 26, 2021
2:00 PM PST
Zoom

Molecules in quantum motion

In order to fully understand the nature of chemical reactions and molecular properties, 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 and nuclear dynamics. 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 interaction of molecules with extreme short and intense light pulses on an attosecond time scale. I will demonstrate how these simulations provide new insight into complex experimental results.

Please contact nikke@chem.ucla.edu for additional information.