



CHEMISTRY &  
BIOCHEMISTRY

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# CHEMISTRY & BIOCHEMISTRY SEMINAR SERIES: Multilayer Multiconfiguration Time-Dependent Hartree Theory

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## Abstract:

The multilayer multi-configuration time-dependent Hartree (ML-MCTDH) theory is a powerful tool to simulate quantum dynamics for large systems. This rigorous quantum approach is based on an efficient representation of the functional in a time-dependent variational calculation, which iteratively or recursively expand the wave function in several (or many) dynamically contracted layers. Mathematically, the expansion is equivalent to hierarchical Tucker tensor decomposition, although the latter usually employs a binary tree structure. A special skewed tree form is called the tensor train in mathematics and matrix product states in physics. In this talk I will discuss the general feature of the theory, the scaling of the method, the relation to a few other tensor contraction schemes, and application of the theory to some model reactions that have interesting many-body quantum effects.

## About the Speaker:

Haobin Wang received his BSc. from Department of Modern Chemistry (now Chemical Physics), University of Science and Technology of China in 1991. He then did his graduate study at Wayne State University, Detroit, Michigan from 1992-1996 under the supervision of William L. Hase. Afterwards he carried out postdoctoral work with William H. Miller at University of California-Berkeley. He was an Assistant Professor of Chemistry at New Mexico State University from 2001 to 2005, Associate Professor 2006-2010, and has been Professor there since 2011. In 2014, he became the chair of the Chemistry Department at University of Colorado Denver. Dr. Wang's research has focused on developing accurate theoretical methods and practical computational techniques to simulate quantum dynamics for large many-body systems. His research interests also include developing classical and semiclassical methods for dynamical simulations. He received the Career award from the National Science Foundation. He will also be the 2025 Romberg Visiting Professor at University of Heidelberg.

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