"FROM ELECTRONIC AND VIBRATIONAL STRUCTURE TO QUANTUM DYNAMICS WITH MATRIX PRODUCT STATES"

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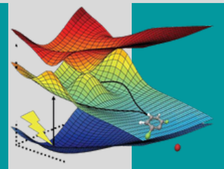
with the words "Markus Reiher – Virtual" on the "subject"
Deadline: November 04, 2021 (Thursday), 06pm (BRT time)



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ABSTRACT

From Electronic and Vibrational Structure to Quantum Dynamics with Matrix Product States

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Tensor network states and in particular matrix product states, which can be efficiently optimized with the density matrix renormalization group algorithm (DMRG), turned out to be a versatile and efficient way to parametrize a many-particle wave function [1], which otherwise suffers from the curse of dimensionality in many-particle quantum mechanics. We have developed a second-generation, i.e., matrix product operator based DMRG program [2], which allows for a fast implementation of new Hamiltonians. For instance, we were able to quickly turn the 'fermionic' program for electronic structure problems into one that can treat vibrational structures [3] and even quantum dynamics [4]. Already these pilot developments turned out to be on a par with the best traditional methods of quantum chemistry. We were able to drive these calculations in a fully automated manner by developing the first protocol that enables the fully automated selection of active orbital spaces [5] that was later turned into the only software available for this purpose [6]. Other advancements concern the development of transcorrelated methods [7] and multi-particle quantum theories [8]. In my talk, I will present a basic introduction to these approaches and then demonstrate their power at challenging chemical problems.

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