Title: High performance ab initio density matrix renormalization group for strongly correlated electrons

Authors: Huanchen Zhai, Zhi-Hao Cui, Tianyu Zhu, Henrik R. Larsson, Seunghoon Lee, Garnet Kin-Lic Chan

Abstract:

Over the last decade, the Density Matrix Renormalization Group (DMRG) algorithm has been established as a reliable method for treating systems with strongly correlated electrons. Recently we have made efforts on pushing DMRG towards a wider range of applications, by integrating it with (i) conventional quantum chemistry methods, such as multireference configuration interaction and n-electron valence state perturbation theory, and (ii) novel ab initio quantum embedding methods, such as density matrix embedding theory and dynamical mean field theory. For this purpose, we have developed a modular and highly scalable ab initio DMRG code with the support of property calculations such as reduced density matrix, Green's function, and spin-orbit coupling. We illustrate how this new computational tool can help us understand the strongly correlated systems at the ab initio level.