

Towards rigorous *ab initio* quantum embedding for realistic systems using Green's function theory

Tran Nguyen Lan¹, Alexei Kananenka¹, Alexander Rusakov¹, and Dominika Zgid¹

¹Department of Chemistry, University of Michigan, Ann Arbor, MI 48109

The self-energy embedding theory (SEET) is a QM/QM Green's function embedding technique recently developed in our group that allows us to treat systems containing both strongly and weakly correlated electrons. In SEET, the strongly correlated electrons described by a non-perturbative expensive and accurate method are embedded in the self-consistent field coming from the weakly correlated electrons described by a relatively cheap perturbative method. SEET is theoretically rigorous and its accuracy can be improved either by increasing the perturbation order or enlarging the number of orbitals treated by the accurate method. SEET was recently applied to the 2D Hubbard lattice and small molecular examples showing promising results. In this talk, I will give a general overview of recent developments necessary to make SEET applicable to realistic molecular and periodic systems.