

Ab initio cavity quantum electrodynamics with equation-of-motion coupled-cluster theory

Quantum electrodynamics coupled-cluster (QED-CC) theory is an ab initio many-body approach to modeling the electronic structure of a molecule strongly coupled to an optical cavity. The dipole moments of the molecule and resonant photons in the cavity couple to form a polariton, a hybrid light-matter state. For the discovery of novel chemistry using polaritons, a robust theoretical framework is necessary to understand the mechanisms behind reactions within a cavity. We present a scalable C++ implementation of QED-CC, realized with the tensor framework TiledArray, that can generate one- and two-particle reduced density matrices and utilize equation-of-motion QED-CC (EOM-QED-CC) to predict excited state properties of hybrid light-matter states.