Coupled-cluster methods for strong light-matter interactions

A. Eugene DePrince, III
Florida State University

Strong coupling of photonic and molecular degrees of freedom can lead to the formation of hybrid light-matter states known as polaritons that can exhibit dramatically different properties relative to the original uncoupled states. A fundamental understanding of the principles that govern polariton formation and manipulation is desirable, as such knowledge can facilitate light-mediated control over chemical transformations. Cavity quantum electrodynamics (QED) coupled-cluster (CC) theory has recently emerged as a powerful approach for the description of cavity-induced effects in many-electron systems. I will discuss the application of equation-of-motion (EOM) QED-CC theory to cavity-bound molecular systems, using both excitation energy and electron attachment variants of EOM-QED-CC.