Exploring Photon-Induced Electron Correlations: Quantum Electrodynamics Coupled-Cluster Theory for Ground and Excited States

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Quantum Electrodynamics (QED) Coupled-Cluster (CC) theory[1,2] serves as a powerful computational framework for accurately predicting the electronic structure of quantum systems while incorporating the effects of photon-electron interactions.

We will discuss the theoretical foundations of the non-relativistic QED-CC approach, emphasizing its treatment of photon-matter interactions within the framework of quantum electrodynamics. Furthermore, we plan to elucidate the computational details of our implementation, encompassing algorithmic strategies and numerical techniques.

Additionally, we aim to demonstrate the efficacy of the QED-CC method in accurately predicting ground and excited state properties by conducting benchmark calculations on selected molecular systems. Our emphasis will be on highlighting the significant role of photon-electron interactions in governing electronic structures.

This heterogeneous parallel implementation, developed by us, provides a promising avenue for studying very large quantum systems with a high degree of accuracy influenced by electromagnetic fields. It promises to illuminate their electronic properties, surpassing the constraints of traditional non-relativistic quantum chemistry methodologies.

1. Tor S. Haugland, E Ronca, Eirik F. kjonstad, A. Rubio, and H. Koch, Phys. Rev. X, **10**, 041043, (2020).
2. M. Ruggenthaler, D. Sidler, and A. Rubio, arXiv preprint arXiv:2211.04241 (2022).