

## Coupled cluster theory for molecular polaritons

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I will present our recently developed *ab initio* correlated approach to study molecules that interact strongly with quantum fields in an optical cavity. Quantum electrodynamics coupled cluster theory (QED-CC)<sup>1</sup> provides a nonperturbative description of cavity-induced effects in ground and excited states. Using this theory, we show how quantum fields can be used to manipulate charge transfer and photochemical properties of molecules. We propose a strategy to lift electronic degeneracies and induce modifications in the ground-state potential energy surface close to a conical intersection. Cavity-induced modulation of intermolecular interactions are also discussed.<sup>2</sup>

1. Tor S. Haugland, Enrico Ronca, Eirik F. Kjørstad, Angel Rubio, and Henrik Koch, Phys. Rev. X **10**, 041043 (2020).
2. Tor S. Haugland, Christian Schäfer, Enrico Ronca, Angel Rubio, and Henrik Koch, arXiv:2012.01080 [physics.chem-ph]

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