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Chemistry and photochemistry in the strong coupling regime - from single molecules to ensemble of molecules

Wednesday 4 October 2023 09:40 (40 minutes)

The theoretical description of molecular polaritons and their properties is still subject to many open questions. In the past years we studied a variety of effects, such as dissipation, to determine its influence on the photochemistry. More recently we have implement Hartree-Fock with the cavity Born-Oppenheimer approximation to investigate the multi-molecule effects in the electronic ground state. Here, we have identified the dipole self energy contributions as a new mechanism to mediate inter-molecular interactions.

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Session Classification: Morning session and closing remarks