Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

Tuesday, December 3rd, 2019 – 14:00 pm
CFEL Seminar room IV (Bldg. 99)

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Coupled cluster theory with applications to conical intersections and quantum electrodynamics

I will review different aspects of coupled cluster theory with focus on recent developments. In particular, similarity constrained coupled cluster theory[1] for conical intersections and nonadiabatic dynamics, pump-probe simulations using time-dependent coupled cluster theory[2] and coupled cluster theory for strong light-matter interactions (Cavity QED chemistry).[3] These developments are all carried out in the framework of a new electronic structure program eT, based on a highly efficient algorithm for the Cholesky decomposition of two-electron integrals.[4]

1. E. F. Kjønstad and H. Koch, J. Phys. Chem. Lett. 8, 4801 (2017)
2. A. Balbi, A. Skeidsvoll and H. Koch (to be submitted)
3. T. S. Haugland, E. Ronca, E. F. Kjønstad, A. Rubio, and H. Koch (to be submitted)
4. S. D. Folkestad, E. F. Kjønstad and H. Koch, J. Chem. Phys. 150, 194112 (2019).

Host: Simone Latini, Angel Rubio

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