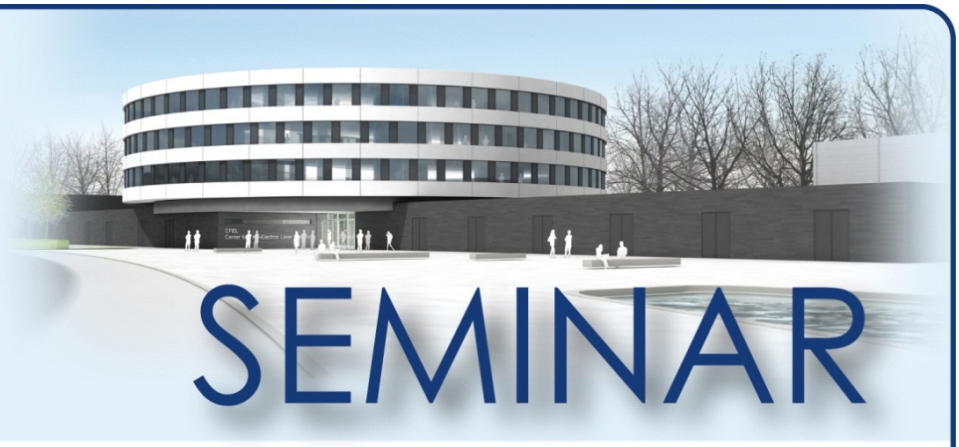
CFEL SCIENCE



SEMINAR

21st May 2025 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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A quantum chemistry perspective on many-body electronic structure methods

In recent years, many-body electronic structure methods originating from theoretical condensed matter physics have been adopted with great success in quantum chemical applications. Similarly, many-body techniques from quantum chemistry are routinely applied in theoretical condensed matter physics. This exchange of many-body methods has resulted in a broad interest in gaining a deeper understanding of their interconnections. In this talk, I will present such a connection for the G0W0 method and the Equation-Of-Motion (EOM) Coupled Cluster (CC) approach for charged excitations [1]. Based on this connection, a practical, frequency-free G0W0 approach [2] and analytic nuclear gradients will be presented [3]. Furthermore, I will discuss how the diagrammatic structure of CC theory allows to get microscopic insights into electronic phase transitions in quantum materials [4].

[1] J. Tölle and G. K.-L. Chan, *J. Chem. Phys.* **158**, 124123 (2023).

[2] J. Tölle and G. K.-L. Chan, *J. Chem. Phys.* **160**, 164108 (2024).

[3] J. Tölle, *J. Phys. Chem. Lett.* **16**, 3672 (2025).

[4] Z. Cui *et al.*, *Nat. Commun.* **16**, 1845 (2025).

Host: Robin Santra – CFEL-DESY Theory Division