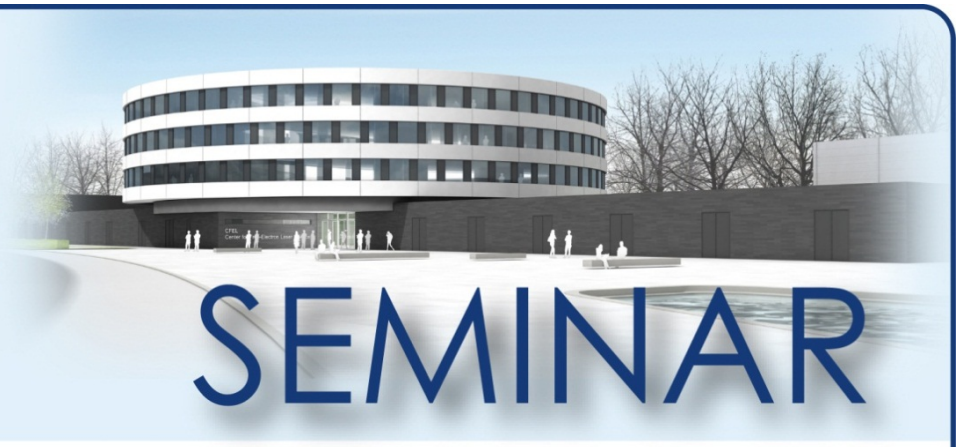
CFEL SCIENCE



SEMINAR

2nd March 2022 - 2:00 p.m.

Virtual meeting room in ZOOM (ID: 895 1951 2902 / PW: 925239)

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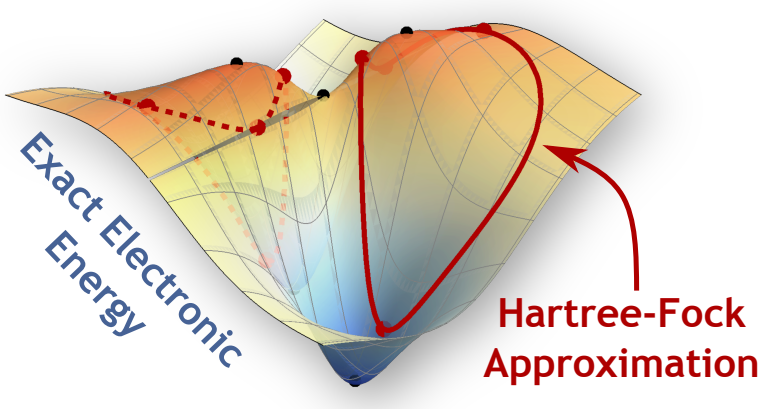
Energy Landscape of State-Specific Electronic Structure Theory

Electronic excited states play an essential role in photochemical processes throughout chemistry. As higher-energy eigenstates, excited states can be difficult to accurately describe using theoretical techniques. One particularly appealing approach is to search for higher-energy mathematical solutions to ground-state methods. These state-specific approximations can accurately describe challenging electronic excitations that involve relaxation of the electron density. However, the global structure of the corresponding electronic energy landscape remains largely unexplored. In this talk, I will introduce a geometric perspective on the energy landscape of exact electronic structure theory. On the exact energy landscape, ground and excited states form stationary points constrained to the surface of a hypersphere. The connectivity and properties of exact stationary points are investigated, and the square-magnitude of the exact energy gradient is shown to be directly proportional to the Hamiltonian variance. I will then explore how approximate methods can be understood through the landscape perspective, highlighting some of the challenges faced by practical state-specific optimization algorithms.



Host: Robin Santra – CFEL-DESY Theory Division