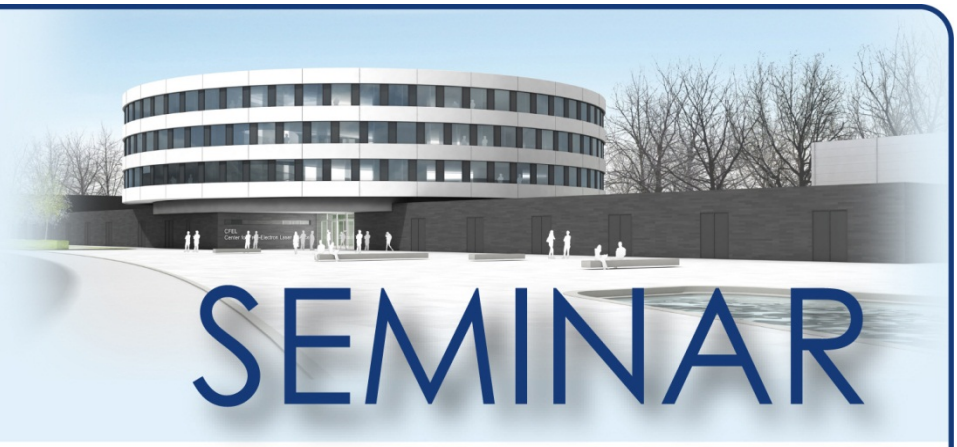
CFEL SCIENCE



SEMINAR

13 June 2024, 10:00–11:00h
CFEL (Bldg. 99) seminar room I+II

Stephan Sauer

Department of Chemistry, University of Copenhagen

Hybrid Quantum Chemistry on NISQ Quantum Computers

The process of rational design of tailor-made molecules possessing desired and specific properties may be brought to revolution, if the relevant molecular properties can be accurately predicted on a reasonable time scale. Even if the necessary quantum chemical methods to achieve such molecular property calculations are well known to quantum chemists, carrying out these calculations on classical computers for large biological molecules in their natural environments is today too slow, if not impossible. This scenario could, however, completely change when large-scale quantum computers become available. They are expected to provide the opportunity to more accurately calculate the outcomes of complex chemical and biochemical processes. Before this realization, however, significant challenges need to be overcome since current quantum chemical software cannot simply be ported to quantum computers. Thereby, specific methodological and algorithmic developments tailored for quantum computers are thus in high need in order to facilitate the transition of molecular property calculations from classical to quantum computers.

This is exactly the goal of our research project supported by the Novo Nordisk Foundation. In this presentation, I will discuss the specific types of quantum chemical methods and calculations we are currently trying to implement on quantum computers and what kind of results we can achieve with them already today.

Host: Jochen Küpper/ CFEL Molecular and Ultrafast Science Seminar