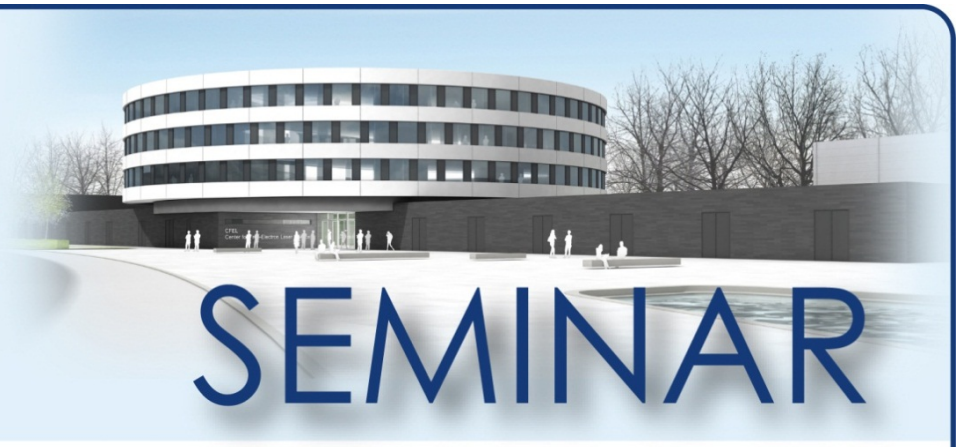
CFEL SCIENCE



SEMINAR

9th September 2020 - 2:00 p.m.

Virtual meeting room in ZOOM (ID: 953 3225 2947 / PW: 598731346)

Michael Obermeyer

Center for Free-Electron Laser Science, DESY, Germany

Excited-state SCF convergence failures: characterization and resolution

For the interpretation of many x-ray free-electron laser experiments a detailed understanding of the radiation damage is crucial. In this context, the ab-initio framework XMOLECULE has been developed to investigate the contribution of molecular effects to the radiation damage. For modelling the x-ray ionization dynamics, electronic states due to sequential multiple x-ray absorption have to be calculated, which involves a huge number of highly excited states. For the efficient calculation of these electronic states the self-consistent-field (SCF) method is used in combination with the maximum overlap method. Already for a small molecule like carbon monoxide (CO) SCF convergence cannot be achieved for all cases. The number of convergence failures increases dramatically for larger molecules. This work characterizes SCF failure cases for CO at fixed geometry. A thorough understanding of why such failures occur and how they are related to specific methodological choices is revealed. From these insights, a strategy is proposed to overcome cases of convergence failures in CO, that promises to solve a large number of failure cases also in larger molecules.

Host: Robin Santra – CFEL-DESY Theory Division