Within the scope of this project, you will learn about novel molecular materials for solar energy harvesting and work within the DTU-based Atomic Simulation Environment (ASE) to help extracting information from huge datasets (30TB+) from X-ray Free Electron Lasers (XFELs).

The efficiency, selectivity, and rate of chemical reactions depend crucially on the environment in which the reaction takes place. Solvation, the local organization of the solvent molecules around a solute, has a central role in the description of condensed phase chemical properties. Simulations including solvation play a crucial role in predicting experimental outcomes and supporting the interpretation of experimental data[1,2].

With this project you will be on the front line of method development- and application, working in close collaboration with experimentalists in the Molecular Movies group of the NEXMAP section, expanding the understanding of the chemical reactions recorded with sub-picosecond time resolution at an XFEL. Your main task will consist of finding and employing the best overall model for simulating the ground- and excited state dynamics of a triple-metal centered complex in solution, which cannot be modelled even qualitatively by common/traditional ab initio methods, when solvation is required. If successful this would represent a first within the field. It will teach you to work with- and develop within an open-source, python-based atomic manipulation environment, used at universities and at companies around the world, and also give you general knowledge of the workflow of large-scale programming efforts.

After a discussion about which approach excites you the most and fits your previous experience best, we will together decide your concrete tasks:

- **The Quantum Chemical Way:** Investigate what ab initio model(s) can successfully be used to describe the complex in solution, investigating the effects of:
  - Density functionals
  - Dispersion approximations
  - Basis sets

- **The Force Field Way:** Develop and employ a molecular-dynamics restraint methodology that ameliorates the effects of shortcomings of the ab initio potentials on the structure, while not affecting dynamics of atoms internally in the complex.

- **The DFT-Development Way:** Test the possibilities of utilizing additional external potentials in the Kohn-Sham Hamiltonian, tuned to match experimental results.

**METHODOLOGY**

DFT: GPAW, CP2K, ORCA. OpenMM, AMBER. General: Python, ASE,

**PREREQUISITES**

Programming experience (preferably python) needed. Experience with either DFT simulations and/or classical force-field dynamics preferred.

**REFERENCES:**

  Dohn, A. O.; Hartsock, R. J.; Nelson, S.; Glownia, J. M.; Lemke, H. T.; Christensen, M.; Gaffney, K. J.; Henriksen, N.
  E.; Møller, K. B.; Nielsen, M. M. Ultrafast X-Ray Scattering Measurements of Coherent Structural Dynamics on the