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Professor

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Research

My field of research is theoretical and computational physical chemistry with emphasis on chemical dynamics. Research topics include quantum theory, the quantum-classical boundary, reaction dynamics and ultrafast time-resolved experimental techniques.

Collaborators are both theoretical and experimental groups at DTU Chemistry and Physics, University of Copenhagen and in France, South Korea, Spain, and USA, and Synopsys QuantumATK Team in Copenhagen.

Most recent scientific publications:

- X-ray transient absorption reveals the ^1A_u ($n\pi^*$) state of pyrazine in electronic relaxation. *Nature Commun. 12, 5003, 2021*
- Trajectory surface-hopping photoinduced dynamics from Rydberg states of trimethylamine *Phys. Chem. Chem. Phys. 23, 10964, 2021*
- An assessment of different electronic structure approaches for modeling time-resolved x-ray absorption spectroscopy. *Struct. Dyn. 8, 024101, 2021*

Relevant courses:

- DTU Chemistry: 26263 - *Molecular electronic structure methods*
- DTU Chemistry: 26236 - *Advanced Physical Chemistry*
- DTU Physics: 10302 - *Electronic Structure Methods in Material Physics, Chemistry and Biology*
- DTU Compute: 02450 - *Introduction to Machine Learning and Data Mining*
- KU Chemistry: NKEA07016U - *Computational Chemistry*

QuantumATK Student Project

Machine Learning Based Large-Scale Prediction of Physical & Chemical Properties

Atomistic simulations with QuantumATK are used in semiconductor, battery, and other materials R&D across a broad range of high-tech industries to predict material physical and chemical properties, such as electronic, structural, optical, thermal, etc. Modeling with QuantumATK reduces development time and cost by down-selection of promising material candidates with desired properties prior to going to the lab and dealing with expensive and possibly hazardous chemicals with unknown properties and behavior.

Density Functional Theory (DFT) atomistic approach is widely applied in predicting these properties accurately for any element in the periodic table in any kind of atomic arrangement, without the need for experimental input parameters. However, DFT simulations are computationally rather expensive and thus scanning of thousands of materials for target properties could take a long time. Machine Learning algorithms, such as Neural Networks, could highly reduce the computational cost of such a large-scale screening.

The goal of this project is to train Machine Learning algorithm(s) with calculated DFT data using QuantumATK for a selected dataset of materials (primarily, molecules). An essential part of this project will be to demonstrate that the trained Machine Learning algorithm can reliably and efficiently predict selected physical and chemical properties of a large pool of new materials that share some common composition and structural features with materials present in the selected dataset.

Benjamin Fogstrup Grundahl
R&D Engineer,
Synopsys QuantumATK, Copenhagen
MSc from DTU Chemistry, 2020

"I studied my master at DTU Chemistry where I did my thesis in collaboration with Synopsys QuantumATK implementing a solvation model called COSMO. It was a great experience and opportunity to challenge myself in a 'real-life' project while knowing that both DTU and Synopsys QuantumATK supported me if I needed any help. I also had the chance to discuss the project with the people working at Synopsys QuantumATK which was a fantastic learning."

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https://www.synopsys.com/quantumatk.html