ChE-701

Advanced simulations of solar cell devices

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Cursus	Sem.	Type
Chemistry and Chemical Engineering		Opt.

Language of teaching	English
Credits	1
Session	
Exam	Oral presentation
Workload	30h
Hours	**27**
Courses	12
Exercises	15
Number of positions	

Frequency

Every year

Remark

Next time Spring semester 2025

Summary

State-of-the-art solar cells. Quantum and classical simulation techniques applied to perovskite solar cells (software: CP2K, QE, LAMMPS,GAUSSIAN). Parametrization of interatomic machine learning potentials using ab initio simulations.

Content

The course aims to provide a brief overview of different solar cell technologies, with a focus on direct and indirect perovskite-based solar cells (PSCs).
The aim of the course is to acquaint students with state-of-the-art quantum and classical simulation techniques applied to PSCs, with the objective of performing high-level simulations to unravel the physical-chemical mechanisms underlying the possible improved performance and stability of PSC devices. The course will also provide a solid introduction to how to develop reliable classical force fields for complex multi-component systems. The topic of interatomic potentials with machine learning (ML) will also be addressed.
An introduction to the main experimental techniques for characterizing PSCs will also be provided, to understand which quantities are most important and how to compare theoretical results with experimental ones.
The course is divided into three modules, starting with a brief introduction to the physical, electronic and optical properties of solar cell devices.
1. PSC characterization: introduction to the main experimental characterization techniques (I-V curve, PLQY, PL spectra, TRPL, XRD, NMR). Emphasis will be placed on how to use this information to set up meaningful simulation protocols.
2. Simulation of PSC devices: students will become familiar with different quantum (Quantum Espresso, CP2K, Gaussian) and classical (LAMMPS, AMBER) simulation software applied to perovskites, different hole transport layers (HTL) and electron transport layers (ETL), also in the case of interaction with passivating molecules. The modeling of perovskite/ETL(HTL) interfaces in the presence/absence of additives will also be addressed. Particular attention will be paid to the simulation of optoelectronic properties (band gaps, band alignment, exciton binding energy, etc.) in the presence/absence of additives.
3. Force field development: in most cases, the size of the system and/or the physical-chemical mechanisms investigated require a number of atoms and/or timescales that can only be achieved with classical MD. In this case, it is essential to have accurate force fields based on ab initio simulations to be sure of correctly capturing all interactions of the system. Students will learn the basic concepts of force field development (including machine learning interatomic potentials) from ab initio data. They will also learn how to parameterize force fields in the presence of composite systems, such as additives and perovskites.

Note

Introduction
1- Introduction to the solar cell design (1h)

2- Main experiments for solar cell characterization (2h)
Quantum
3- Introduction on electronic structure calculations with the focus on solar cells and periodic systems
4- Introduction on perovskites and influence of the most common defects on the electronic properties and stability
5- How to check surface stability, finite temperature simulations
6- Band alignment, transport properties, molecular orbitals
7- ETL/AL/HTL interfaces
Classical
8- Parametrizing the system/adjusting the force field
9- Conformational sampling and system equilibration for getting good starting point for QM
10- Mechanistic properties (young modulus etc.)
ML
11- How to efficiently parametrize a ML force field
12- Application to solar cells

Keywords

Photovoltaics, perovskite-based solar cells, atomistic simulations, force field development

Learning Prerequisites

Required courses

Quantum mechanics, classical molecular dynamics

Learning Outcomes

By the end of the course, the student must be able to:

- Distinguish between different simulation techniques, choose and design the simulation protocol according to the desired purpose

Assessment methods

Oral presentation (exposé)

Resources

Moodle Link

- https://go.epfl.ch/ChE-701