Computational modelling of materials for energy applications

Subject area: Physics

University:	DTU
Level:	MA all years, PhD
Teaching mode:	completely online, not time-specific
Instructor(s):	Ass. Prof. Ivano E. Castelli; Ass. Prof. Piotr de Silva

Short description

In this course, you will acquire basic knowledge of computational methods, in particular Density Functional Theory (DFT), and apply them to design novel materials related to energy applications using high-throughput and machine learning techniques. This course combines lectures on DFT, machine learning, and materials design with exercises and tutorials. The examples will cover different applications within the challenges of energy conversion and storage.

Full description

In this course, the student will get an introduction to Density Functional Theory (DFT) as one of the most used computational tools to study fundamental processes in materials for energy conversion and storage (batteries, nanocatalysts, fuel cells, photovoltaics, etc.). In the first half of the course, the students will learn the basics of the atomistic description of materials and electronic structure as well as the fundamentals of DFT. The second part is more practical, and the students will first learn which properties can be calculated using DFT and how to bridge these quantities with the measured properties from experiments as well as how to implement methodologies to automate and accelerate the design of novel materials. The course focuses on the application of DFT through dedicated exercises, with limited technical details about the methodology used.
The course is composed of eight lectures, each with three to five video lectures, quizzes and exercises. A weekly one-hour live chat and a forum will be set up for discussion and feedback. In the final project, the students will use the tools described in the course to predict the properties of energy materials. Examples from the previous final projects are the investigation of materials for light-harvesting and the study of properties of 2D materials. The final project will be proposed depending on the interests of the students.
More details on the course can be found here:
https://kurser.dtu.dk/course/2021-2022/47335

Learning outcomes

A student who has met the objectives of the course will be able to:
- Describe the basics of computer simulations with a focus on Density Functional Theory and the quantities that can be calculated
- Describe the physics behind key applications for energy materials
- Interpret and adapt computer scripts for calculating physical properties of materials
- Identify descriptors for an accelerated materials discovery approach
- Understand how to connect experimental results and simulations
- Understand and apply machine learning approaches for materials design
- Apply high-throughput and machine learning techniques to a given data set to find novel materials
- Perform high-level computer simulations of identified materials for energy applications
- Identify problems and solutions related with computer simulations and materials discovery

General information

Contact hours per week:	1 hour webinar each week plus online forum
Total workload:	140 (in student hours for the whole course)
ECTS credits:	5
Language:	English
Course start date:	29 August 2022
Course end date:	09 December 2022
Add. info about start date:	
Weekly teaching day/time:	
Time zone:	CET (Denmark, Germany, France, Netherlands, Switzerland, Czech Republic)
Further information:	
Prerequisites:	Basic concepts from physical chemistry and/or condensed matter physics are needed for the present course. No previous coding experience is required, although it is advantageous.
Activities and methods:	Lectures, Exercises, Computer exercises
Presence on campus:	Not required

Final examination

Form:	oral
Date:	

Location/format:	online
Re-sit possibility:	no
Transcript available:	shortly after the examination
Add. info/requirements:	Oral examination consisting of a 10 minutes oral presentation of the final project plus 15 minutes for questions on the project and course curriculum.

Registration

To register for this course, follow the registration requirements of your **home university** as specified here: www.euroteq.eu/courses-registration.

Administration

Number of places:	20
Minimum participants:	
Internal course code:	47335
Contact:	Ivano E. Castelli (ivca@dtu.dk)

This course is part of the EuroTeQ Engineering University joint course catalogue 2022/2023. This is a collaborative activity of the partner universities DTU, L'X, TU/e, TalTech, CTU, TUM as well as Technion. Students from these universities can participate in the offered courses. It is the responsibility of the student to check if you fulfil the requirements to participate in a specific course. Students are also advised to check with their home institution how to get recognition of the ECTS credits gained in courses of the EuroTeQ course catalogue. For further information about EuroTeQ Engineering University, visit www.euroteq.eu or get in touch with the above-mentioned point of contact.