

PhD position in Machine Learning Quantum Mechanics for Materials Science

The section for Computational Atomic-scale Materials Design (CAMD) at the Technical University of Denmark (DTU), is seeking an outstanding and highly motivated candidate for a PhD position within the area of artificial intelligence (AI) for prediction of electronic properties of crystalline materials.

The successful candidates will develop and use AI-based algorithms for predicting electronic properties, e.g. formation energies, electronic band structures, and optical absorption spectra, of crystalline solids exploiting the vast amount of materials data provided by existing open databases including the Computational Materials Repository developed at and maintained by the group. In the last phase of the project the developed methods will be used to explore novel structure-property relations and screen vast hypothetical materials spaces (in terms of chemical composition and crystal structure) to identify new candidate materials for opto-electronic applications.

CAMD offers an international and scientifically stimulating working environment at the Department of Physics, DTU, located in the northern Copenhagen area. The group has strong connections to local experimental groups within the VILLUM Center for the Science of Sustainable Fuels and Chemicals

<http://www.camd.fysik.dtu.dk/> and the Center for Nanostructured Graphene.

<http://www.v-sustain.dtu.dk/> <http://www.cng.dtu.dk/>

Substantial computational resources are available for the project through the DTU-supercomputer facility Niflheim. The position is part of a strategic alliance with Aalto University and will involve visits to the group of Prof. Patrick Rinke.

<https://wiki.fysik.dtu.dk/niflheim/>

Qualifications

The successful candidate will have obtained excellent grades in his/her Bachelor and Master educations. Knowledge of machine learning and quantum mechanics is an advantage as is programming experience (e.g. Python, C, C++). Furthermore, the candidate should be highly motivated and willing to work as part of a team. Good communication skills in both spoken and written English, are a requirement.

Approval and Enrollment of PhD Students

The scholarships for the PhD degree are subject to academic approval, and the candidates will be enrolled at the Physics PhD School at DTU. For information about the general requirements for enrollment and the general planning of the scholarship studies, please see PhD at DTU. <http://www.dtu.dk/english/education/phd>

Assessment

The assessment of the applicants will be made by Professor Kristian S. Thygesen.

We offer

DTU is a leading technical university globally recognized for the excellence of its research, education, innovation and scientific advice. We offer a rewarding and challenging job in an international environment. We strive for academic excellence in an environment characterized by collegial respect and academic freedom tempered by responsibility.

Salary and appointment terms

The appointment will be based on the collective agreement with the Danish Confederation of Professional Associations. The allowance will be agreed upon with the relevant union. The period of employment is 3 years. The position is available immediately, and must start in 2019.

The position, which involves a limited teaching obligation, includes salary and travel grants covering the three years it takes to obtain a PhD degree at a Danish university. Salary level is approximately 50.000 Euro/year incl. pension.

You can read more about career paths at DTU here.

<http://www.dtu.dk/english/about/job-and-career/working-at-dtu/career-paths>

Further information

Should you have any queries regarding the positions, please contact Professors Kristian S. Thygesen, thygesen@fysik.dtu.dk.

Application

Please submit your online application no later than 1 August 2019 (local time). Applications must be submitted as one PDF file containing all materials to be given consideration. To apply, please open the link "Apply online", fill out the online

application form, and attach all your materials in English in one PDF file. The file must include:

- A letter motivating the application (cover letter)
- Curriculum vitae
- Grade transcripts and BSc/MSc diploma
- Excel sheet with translation of grades to the Danish grading system (see guidelines and Excel spreadsheet here)
http://www.dtu.dk/english/Education/phd/Applicant/Pre_acceptance-1-

Candidates may apply prior to obtaining their master's degree but cannot begin before having received it.

Applications and enclosures received after the deadline will not be considered.

All interested candidates irrespective of age, gender, race, disability, religion or ethnic background are encouraged to apply.

DTU is a technical university providing internationally leading research, education, innovation and scientific advice. Our staff of 6,000 advance science and technology to create innovative solutions that meet the demands of society, and our 11,200 students are being educated to address the technological challenges of the future. DTU is an independent university collaborating globally with business, industry, government and public agencies.