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UNIVERSITY OF
LUXEMBOURG

Doctoral researcher (PhD student) in Quantum machine learning for reactivity

Luxembourg,
Luxembourg

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JOB DESCRIPTION

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The **University of Luxembourg** aspires to be one of Europe's most highly regarded universities with a distinctly international and **interdisciplinary character**. It fosters the cross-fertilisation of **research** and **teaching**, is relevant to its country, is known

ABOUT THE EMPLOYER

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ACADEMIC STORIES



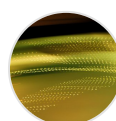
Quantum Computers Will Change Everything. Including Our Security Needs.

"Certain quantum algorithms have been proposed that will be able to break all of our security today."



Tracking the Curve: Analyzing the Emotional Response to COVID-19

Professor Xiangliang Zhang is using machine learning to track the changing emotional response to the global crisis.



Bringing Quantum Computers Closer to Reality

Stacey Jeffery of CWI and her collaborators recently made a major breakthrough in quantum computing algorithms.

worldwide for its research and teaching in targeted areas, and is establishing itself as an innovative model for contemporary European Higher Education. It`s core asset is its well-connected world-class academic staff which will attract the most motivated, talented and creative students and young researchers who will learn to enjoy taking up challenges and develop into visionary thinkers able to shape society.

The Faculty of Science, Technology and Medicine (FSTM) contributes

multidisciplinary expertise in the fields

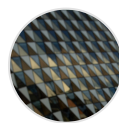
of **Mathematics, Physics, Engineering, Computer Science, Life Sciences** and **Medicine**.

Through its dual mission of teaching and research, the FSTM seeks to generate and disseminate knowledge and train new generations of responsible citizens, in order to better understand, explain and advance society and environment we live in.

The University of Luxembourg is looking for a doctoral candidate to start working on the project "Quantum machine learning for reactivity" funded by the H2020-MSCA-ITN-2020 (<http://ai-dd.eu/>). The application of machine learning (ML) for chemical reaction predictions has recently gained considerable attention in the chemical industry. Although ML models have been developed for the estimation of reactants and/or products of chemical reactions under certain conditions, less emphasis has been

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placed on predicting transition state features. Moreover, a common problem in these works has been the lack of an extensive dataset, restricting the full exploration of the vast chemical reaction space (CRS) defined by reaction type, reactants, products, reaction conditions, transition states, etc. This has also impeded further progress of ML techniques for the understanding of the CRS and the prediction of its components. Hence, this project aims at the design and validation of novel ML-based tools benchmarked on quantum mechanical reference data of pharmaceutically relevant chemical reactions, which can then be used to accurately predict diverse components of the vast CRS emphasizing in transition state features.

The candidate will be integrated into the activities of the Theoretical Chemical Physics group lead by Prof. Alexandre Tkatchenko (www.tcpunilu.com) for the first half of the doctoral studies (18 months) while the second half will be carried out at Janssen Pharmaceutical (Belgium, 18 months). This project will allow the candidate to interact with the scientific staff from some of the world's top universities and pharmaceutical companies.

Your Role

The candidate's tasks include:

- Conducting world-class research in the field of Quantum Machine Learning.

Participating actively in the TCP research group (tcpunilu.com) and the AIDD consortium (<http://ai-dd.eu/>)

Communicating research results in international conferences and journals

Building a strong link to the project partner Janssen Pharmaceutical

Your Profile

We are looking for enthusiastic candidates with a master's degree in Physics, Chemistry, Material Science or Computer Science. Personal initiative, the ability to work independently as well as team-oriented research and language skills (English) are expected. Applications from women are particularly welcome. The same applies to people with disabilities.

Due to the European Commission's eligibility criteria, candidates must not have resided or carried out their main activity (work, studies, etc.) in Luxembourg for more than 12 months in the 3 years immediately before the recruitment date. Compulsory national service, short stays such as holidays, and time spent as part of a procedure for obtaining refugee status under the Geneva Convention are not taken into account.

We offer

A large and dynamic department with an exciting international environment

The chance to work within an excellent consortium for a European Industrial Doctorate

funded by the European Commission

Training in scientific and transferable skills; participation in schools, conferences and workshops

The University of Luxembourg offers highly competitive salaries and is an equal opportunity employer

In Short

Contract Type: 18 months fixed-term contract

Work Hours: Full Time 40.0 Hours per Week

Location: Limpertsberg

Employee and student status

Foreseen starting date: Summer/Autumn 2021

Job Reference: UOL03649

Further Information

Please submit your comprehensive application including

A letter of motivation

A detailed CV

At least two letters of reference

Early application is highly encouraged, as the applications will be processed upon reception. Please apply ONLINE formally through the HR system. Applications by email will not be considered.

The University of Luxembourg embraces inclusion and diversity as key values. We are fully committed to removing any discriminatory barrier related to gender, and not only, in

recruitment and career progression of our staff.

Here's what awaits you at the University

Multilingual and international character. Modern institution with a personal atmosphere. Staff coming from 90 countries. Member of the "University of the Greater Region" (UniGR).

A modern and dynamic university. High-quality equipment. WiFi on campus. Close ties to the business world and to the Luxembourg labour market. A unique urban site with excellent infrastructure.

A partner for society and industry. Cooperation with European institutions, innovative companies, the Financial Centre and with numerous non-academic partners such as ministries, local governments, associations, NGOs ...

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[Addresses, maps & routes to the various sites of the University](#)

Further information

For further information, please contact Dr. Leonardo Medrano Sandonas, at leonardo.medrano@uni.lu, or Prof. Dr. Alexandre Tkatchenko, at alexandre.tkatchenko@uni.lu



JOB DETAILS

Title	Doctoral researcher (PhD student) in Quantum machine learning for reactivity
Employer	University of Luxembourg
Job location	6, rue Richard Coudenhove-Kalergi, L-1359 Luxembourg
Published	October 20, 2020
Application deadline	Unspecified
Job types	PhD
Fields	Quantum Computing , Machine Learning

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University of Luxembourg

Location: Luxembourg,
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PhD-student (Doctoral researcher) in Engineering Science

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