

We are one of the youngest universities in Germany and think in terms of possibilities, not limitations. In the heart of the Ruhr Area, we develop ideas of the future at our 11 faculties. We are strong in research and teaching, in living diversity, as well as in supporting potential. We are highly committed to an educational equality that has earned this name.

The **University of Duisburg-Essen** invites applications for the position of a

Post-doctoral position (f/m/d)
(Payment according to Grade E 13 TV-L)

at the **Faculty of Physics**, Theoretical Physics, Duisburg Campus

Main research topics and duties:

Participation in the research project “**DIMENSION: Determining materials for energy conversion**” with a focus on the development of a research data exchange platform for all projects involved in DIMENSION and the application of machine-learning models to advance the discovery of materials for energy conversion at different system levels.

The typical chain of discovery of active materials is frequently linear in the sense that a set of candidate materials is investigated computationally with the most promising lead compounds being subsequently tested for activity, stability and scalability. The linearity of these tests might lead to an exclusion of compounds that are not top-level for a given property but prove to be top-performers in later stages. The materials discovery can hence be regarded as a highly non-linear optimization problem, with an adaptable objective function. To leverage information of experimental results gained at all individual stages of the project, a research data exchange platform needs to be developed that ensures the interoperability of the heterogeneous experimental and computational data. This requires experience and knowledge of principles in data semantics and ontology applied to real-world data. This platform will then be the basis for machine learning models that guide computations and experiments upstream and downstream to find suitable materials for energy conversion more efficiently, thereby overcoming the linearity of the process.

The successful applicant will be jointly supervised by Dr. Christopher Stein from the Faculty of Physics (Institute for Theoretical Physics) und Dr. Irenäus Wlokas from the Faculty of Engineering (Institute for Combustion and Gas Dynamics – Fluid Dynamics). Communication and exchange with all groups in the DIMENSION project is mandatory and the successful applicant will therefore be located at the NETZ building on the Duisburg campus in close proximity to the other groups.

As part of this postdoctoral researcher position, the successful applicant is offered ample opportunity for further scientific training including the participation in national and international conferences and support with the preparation of grant proposals.

Required qualifications:

Ph.D. in an area relevant to the project with a top-level degree is expected. A very good command of written and spoken English is essential.

Experience with the Python programming ecosystem and detailed background knowledge of common programming paradigms. Some experience with database handling and understanding of basic concepts in materials science and electrochemistry are also required. Due to the interdisciplinary character of the project and the required efficient exchange with several groups from different fields, we expect candidates to have excellent communication skills.

We offer:

- Exciting development potential in the rapidly expanding research fields of machine learning, materials science and energy conversion
- A highly creative, interdisciplinary and international environment with room for own ideas and their realization by means of a sustainable, future oriented technology
- A young, open-minded and motivated team

Expected start of position: May 1, 2022

Contract period: 1 1/2 year

Working time: 100%

Application deadline: 28.04.2022

The University of Duisburg-Essen aims to increase the diversity of its members (see <http://www.uni-due.de/diversity>). It also aims to increase the number of women among its academic staff and therefore encourages women with pertinent qualifications to apply. Women with equal qualifications will be preferred in accordance with state equality laws. Applications of qualified disabled persons in the legal sense of § 2 para. 3 SGB IX are also welcome.

Please submit your application (detailed motivation letter, CV, copy of the Ph.D. certificate, diplomas, transcript of modules taken with grades, a letter of recommendation) quoting reference 259/22 to Dr. Christopher J. Stein, Universität Duisburg-Essen, Fakultät für Physik, Lotharstr. 1, 47048 Duisburg, or, preferably in a single pdf-file, to christopher.stein@uni-due.de.

Information on the faculty and the advertised vacancy is available at:

https://www.uni-due.de/physik/index_en.php

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