

We are a young, innovative university in the middle of the Ruhr Metropolis. Excellent in research and teaching, we think in terms of possibilities instead of limits and develop ideas with a future. We live diversity, promote potential and are committed to educational equality that deserves this name.

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

**Scientific Researcher (f/m/d) at the Faculty of Physics,
Theoretical Physics, Duisburg Campus**

(Payment according to Grade E 13 TV-L)

Main research topics and duties:

Participation in the research project "**CharGeBatCat - Charting** chemical space to generate insight into lifetime-defining processes in **batteries** and **catalysts**" with a focus on the development of density-functional tight-binding methods with explicit spin-dependence and automated parameter optimization. Batteries and (electro)catalysts have become indispensable parts of our everyday lives and industry and they are an important component for a sustainable energy supply. At the same time, the physicochemical processes involved are complex and their details are often not completely understood. This applies in particular to processes that influence the lifetime of these energy systems by adverse side reactions.

Goal of the offered PhD position is to develop and implement a density-functional tight-binding model that explicitly includes the spin density dependence. This development will be augmented by an automated parameter optimization of this semi-empirical model. In combination with other subprojects of this research project, this exploration of the chemical space will allow us to reveal mechanisms that shorten the lifetime of energy materials.

Participation in the preparation of courses, teaching duties and administrative duties are also expected. As part of this graduate position, the successful applicant is offered ample opportunity for further scientific training (culminating in a PhD).

The position is supported by the Ministry of Innovation Science and Research ("NRW-Rückkehrerprogramm" to Dr. Stein).

Required qualifications:

- Completed university studies in physics, chemistry or a related field of at least 8 semesters of standard period of study. A top-level thesis (< 2.0 in the German system) and top-level graded weighted courses are required
- A very good command of written and spoken English is essential
- In addition, knowledge of electronic-structure theory and statistical physics, first experience in the application of DFT programs (Q-Chem, Orca or similar), and programming experience in common languages (C++, Fortran, Python) are desired

We offer:

- a varied, versatile range of tasks
- further education offers
- discounted company ticket for public transport
- opportunity to participate in sports and health programs (university sports)

<u>Expected start of position:</u>	February 1, 2022
<u>Contract period:</u>	3 years
<u>Working time:</u>	75% of a full time employment
<u>Application deadline:</u>	19.12.2021

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 (motivation letter, CV, diplomas, transcript of modules taken with grades, a letter of recommendation) quoting **reference 960-21** 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

<https://www.uni-due.de/en/index.php>

