

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

## **Scientific Researcher (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 "CharGeBatCat - Charting chemical space to generate insight into lifetime-defining processes in batteries and catalysts" with a focus on the development of grand-canonical Monte Carlo methods for the exploration of chemical space in energy materials.

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 identify these processes using a combination of efficient electronic-structure methods and grand-canonical Monte Carlo simulations. In terms of method development, the focus is on the design and implementation of the aforementioned Monte Carlo method. This method will then be used to investigate the stability of several battery systems and, in particular, the formation of the "solid-electrolyte interface" (SEI) under different conditions (surface types, additive addition, etc.). 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 or chemistry of at least 8 semesters. 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
- a company ticket for public transport
- opportunity to participate in sports and health programs (university sports)

**Expected start of position:** August 1, 2021

**Contract period:** 3 years

**Working time:** 75% of a full time employment

**Application deadline:** **25.06.2021**

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 296-21 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](mailto: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/physik/index_en.php)

