

*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

**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 "**CharGeBatCat - Charting** chemical space to **generate** insight into lifetime-defining processes in **batteries and catalysts**" with a focus on the development of embedded cluster models for the simulation of processes 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 materials by adverse side reactions.

The goal of this postdoctoral position is to develop and apply efficient embedded cluster models, that allow the simulation of diverse processes at surfaces. Possible models include DFT-in-DFT embedding or the potential function embedding theory. The focus is primarily on metal surfaces. A second focus will be the coupling of these embedding models to implicit solvation models developed in our group.

Participation in the preparation of courses and teaching is also expected.

As part of this graduate 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.

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

**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
- In addition, knowledge of electronic-structure theory and statistical physics, experience in the application of DFT programs (Q-Chem, Orca, Molcas or similar), experience in the application and/or implementation of embedding models 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)

**Expected start of position:** March 1, 2022

**Contract period:** 31.08.2023

**Working time:** 100%

**Application deadline:** 12.01.2022

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 1011-21** 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)

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