

We are a young, innovative university in the middle of the Ruhr Metropolis. We are strong 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 justice that 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 Chemistry, Theoretical Inorganic Chemistry, Campus Essen.

Main research topics and duties:

Participation in the research project “**Multiscale Modeling to Discover Low-Cost Electrode Materials Based on MXenes for Metal-Air Batteries**” (NRW Return Program Exner). The focus of the work is on the high-throughput characterization of MXenes in aprotic electrolytes for reversible oxygen electrocatalysis in metal-air batteries.

The aim of the advertised position is to identify potential electrode/ electrolyte combinations for MXene-based electrode materials that show sufficient activity and stability in the oxygen evolution and reduction reactions in aprotic solvents. The scientific work aims to transfer existing heuristic screening approaches, originally developed for aqueous electrolytes, to aprotic solvents and to further develop them. Information on these methods can be found in the literature (*ACS Catal.* **2020**, *10*, 12607-12617 & *Chem Catal.* **2021**, DOI: 10.1016/j.checat.2021.06.011).

Participation in the preparation of courses, teaching duties, and administrative duties are expected. As part of this graduate position, the successful applicant is offered ample opportunity for further scientific training (culminating in a PhD). The advertised position is financed with funds from the Ministry of Culture and Science of the Federal State of North Rhine-Westphalia via the NRW Return Program (to Prof. Exner).

Required qualifications:

Completed university degree in chemistry or physics of at least 8 semesters. A good degree (min. 2.0 according to the German grading system) is required. Very good written and spoken English skills are also a prerequisite.

In addition, knowledge in the application of electronic structure calculation (density functional theory, e.g. VASP, WIEN2k, CP2K or SeqQuest) is expected. Experience in the application of ab initio molecular dynamics simulations is desirable, but not necessary. Programming experience or knowledge in the field of (theoretical) electrochemistry is not required but will be considered positively in the application process.

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: October 1, 2021

Contract period: 36 months

Working time: 50% of a full-time employment

Application deadline: August 9, 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 530-21** to Prof. Dr. Kai Exner, Universität Duisburg- Essen,

Fakultät für Chemie, Campus Essen, 45117 Essen. Preferably, compile your application in a single pdf-file and send it via email to kai.exner@uni-due.de.

Information on the faculty and the advertised vacancy is available at: www.uni-due.de

