

*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 Chemistry, Theoretical Inorganic Chemistry, Campus Essen.

**Main research topics and duties:**

Participation in the research project **“Theoretical Investigations of Pentlandites as Earth- Abundant Electrode Materials for Alkaline Water Splitting“** with the focus on the investigation of pentlandites for the electrochemical oxygen evolution reaction.

The oxygen evolution reaction (OER) corresponds to the anodic reaction in water electrolyzers, which convert water into the energy vector hydrogen and oxygen at the cathode and anode, respectively. While the formation of hydrogen at the cathode is a fast two- electron process, the anodic OER is a slow four- electron process, and therefore limits the overall efficiency of electrolyzers. Consequently, cost- effective high- performance OER catalysts need to be developed in order to increase the performance of electrolyzers within the scenario of a sustainable energy economy.

Pentlandite is a common mineral from the mineral class of sulfides and sulfosalts. Experimental investigations have shown that pentlandite- based materials are potential electrocatalysts for the OER in alkaline medium. Yet, the mechanistic processes of the OER on pentlandites are unknown. Knowledge of the reaction mechanism may enable developing pentlandite- based materials with improved catalytic properties for the OER, which thereupon are synthesized and electrochemically characterized by experimental groups.

As part of the advertised position, the reaction mechanism of the OER over iron- nickel- based pentlandites is studied by modern theoretical methods, such as density functional theory as well as ab initio molecular dynamics simulations. To resolve the elementary processes of the OER, the investigated mechanistic pathways are validated by experimental data, such as current- potential curves. Based on the identified reaction steps, the phase space of the pentlandite- based materials is investigated using a heuristic screening approach in order to identify potential high- performance OER catalysts.

The work on the research project includes close collaboration with experimental working groups via the cluster of excellence RESOLV (Ruhr Explores Solvation), funded by the federal government as well as the federal state of North Rhine- Westphalia.

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 advertised position is financed with funds from the RESOLV Cluster of Excellence.

**Required qualifications:**

Completed university studies in chemistry or physics with a master's or diploma degree (Track I) or a bachelor's degree (Track II). To be accepted into the integrated Graduate School Solvation Science (iGSS) of the Cluster of Excellence RESOLV, you must have an excellent degree (grade 1.5 or better in the German system) in chemistry, physics or a related discipline. Very good knowledge of English (level B2, oral and written) is 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:** September 1, 2021

**Contract period:** 36 months

**Working time:** 50% of a full-time employment

**Application deadline:** June 30, 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 432-21** 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](mailto:kai.exner@uni-due.de).

*Information on the faculty and the advertised vacancy is available at: [www.uni-due.de](http://www.uni-due.de)*

