*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 if the collective requirements are met)**

at the Faculty of Chemistry, Theoretical Inorganic Chemistry, Campus Essen.

**Main research topics and duties:**

Participation in the research project **"Comprehending the Oxygen and Chlorine Evolution Reactions over $IrO_2$- Based Electrode Materials on the Atomic Scale"** with the focus on the investigation of iridium- based materials for the electrochemical oxygen and chlorine evolution reactions.

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. In the presence of chloride anions, the chlorine evolution reaction (CER) is a competing side reaction at the anode, which reduces Faradaic efficiency. Knowledge of the reaction mechanism may enable developing high- performance catalysts with selectivity toward either the OER or the CER. The predicted electrode compositions are thereupon synthesized and electrochemically characterized by experimental groups.
As part of the advertised position, the reaction mechanism of the OER and CER over iridium dioxide electrodes is studied by modern theoretical methods, such as density functional theory as well as ab initio molecular dynamics simulations. Based on the identified reaction steps, the selectivity problem of the competing OER and CER is analyzed on the atomic scale to capture the influence of chloride anions on the activity of iridium- based materials for the seawater splitting. Combining this knowledge with heuristic screening approaches may allow identifying high- performance catalysts for the OER or CER.
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:** 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 529-21** 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*

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