

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, 100 %)**

at the Faculty of Chemistry, Theoretical Inorganic Chemistry (located at the campus in Essen).

The working group Theoretical Inorganic Chemistry, headed by Prof. Dr. Kai S. Exner, deals with the theoretical description of catalytic processes at electrified solid/liquid interfaces for electrochemical applications. As part of the Collaborative Research Center/ CRC 247 (Heterogeneous oxidation catalysis in the liquid phase), a position is to be filled that models the electrochemical oxidation of alcohols on cobalt oxides and cobalt ferrites in close cooperation with experimental and other theoretical working groups. The scientific researcher can network well within the SFB 247 and uses these synergies to resolve the elementary processes of alcohol oxidation at the atomic level.

#### **Main research topics and duties:**

Scientific participation in the research project A6 of the CRC 247, which is led by Prof. Spohr and Prof. Exner. The advertised position is part of the Exner group, which focuses on the application of density functional theory (DFT) calculations for the description of electrocatalytic reactions. The Spohr group has many years of expertise in the field of molecular dynamics simulations at electrochemical interfaces. The scientific researcher works closely with the associated scientists of the Spohr group to combine the static, energetic description using DFT with dynamic methods.

Alcohol oxidation is an alternative option to the oxygen evolution reaction (OER) in electrolyzers to produce, besides the cathodic formation of the energy vector H<sub>2</sub>, platform chemicals at the anode. However, the OER is a competing reaction in aqueous electrolytes, and thus, the anodic oxidation of alcohols is inevitably accompanied by a selectivity problem. Selectivity of the competing reaction channels is aimed to be understood at the atomic level and connected to experimental data within the CRC 247. For this purpose, electronic structure calculations in the DFT approximation are used, which are analyzed by descriptor-based approaches. An exemplary overview of the methods used in the Exner group can be found in the literature:

K. S. Exner, *ACS Catal.* **2020**, *10*, 12607-12617.

K. S. Exner, *Angew. Chem. Int. Ed.* **2020**, *132*, 10320-10324.

A. Ivanova, A. Chesnokov, D. Bocharov, K. S. Exner, *J. Phys. Chem. C* **2021**, *125*, 10413-10421.

K. S. Exner, T. Lim, S. H. Joo, *Curr. Opin. Electrochem.* **2022**, *34*, 100979.

S. Razzaq, K. S. Exner, *Electrochim. Acta* **2022**, *412*, 140125.

T. He, K. S. Exner, *Mater. Today Energy* **2022**, *in press*, DOI: 10.1016/j.mtener.2022.101083.

In addition, the scientific researcher will be involved in the implementation of teaching activities or administrative tasks.

#### **Required qualifications:**

Above-average university degree in chemistry or physics of at least 8 semesters. A good degree (at least 2.0 according to the German grading system) is expected. Furthermore, you hold a PhD in theoretical chemistry or theoretical physics, ideally specialized in the field of theoretical electrochemistry. You should have excellent knowledge in at least two of the below areas, ideally in several of them:

- Density functional theory (DFT) calculations with implicit solvation
- Grand canonical approaches to determine adsorption energies
- DFT calculations of magnetic solids and surfaces
- Usage of the program packages VASP and CP2K
- Microkinetic modeling using steady-state approaches

Excellent knowledge of the theoretical fundamentals of electronic structure calculation and excellent programming skills (Python, Java, C++, Wolfram Mathematica, or others) are also expected.

- You have an interest in interdisciplinary research topics
- You can contribute to a team and set new impulses
- You have excellent presentation and communication skills

- You are fluent in German and English
- You have extensive experience in writing scientific texts
- You work in a goal-oriented, structured, and responsible manner
- You are an organizational talent
- You are open to new developments and creative solutions

**We offer:**

- A varied, versatile range of tasks in a research-driven environment with international exchange
- An interesting, responsible job with great creative potential, in which you take upon responsibility and establish networks with other working groups of the CRC 247
- A pleasant and open working atmosphere in a dynamic, young, and intercultural team
- The opportunity for further educational training after the PhD by the development of new scientific focal points
- Family friendliness through flexible and individual care for your children
- Further education offers
- A company ticket for public transport
- Opportunity to participate in sports and health programs (university sports)

**Expected start of position:** January 1, 2023

**Contract period:** 42 months (3 years and 6 months)

**Working time:** 100% of a full-time employment

**Application deadline:** August 29, 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 (motivation letter, CV, diplomas, transcript of modules taken with grades, PhD certificate, a letter of recommendation) quoting **reference XX-YY** to Prof. Dr. Kai Exner, Universität Duisburg- Essen, Fakultät für Chemie, Campus Essen, 45117 Essen. Please 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 CRC 247 and the University Duisburg-Essen is available at:*  
[https://www.uni-due.de/sfbtrr247/](https://www.uni-due.de/sfbtrr247)  
[www.uni-due.de](http://www.uni-due.de)

