Postdoctoral Research Fellowship in Theoretical/Computational Chemistry

One position as Postdoctoral Research fellow available at the Department of Chemistry, Johannes Gutenberg-University, Mainz, Germany (JGU).

The fellowship is for a period of up to 3 years, ending Dec. 31, 2025. Starting date as soon as possible.

Job/ project description:

This project is dedicated to the computational modelling of heterogeneous redox processes at the cathode under the supervision of Prof. Jürgen Gauss, and the co-supervision of Profs. Gregor Diezemann and Michele Cascella. The research is part of the project *ECHELON - Disruptive electrode-electrolyte concepts beyond current scientific limitation*s, funded by the Carl Zeiss Foundation.

The ECHELON project is dedicated to the understanding of all the molecular processes that drive and disrupt electron transfer from the cathodic surface to the reducing substrates, with the aim of designing better catalytic interfaces able to favour such processes, making them accessible at milder conditions (i.e. lower extra potentials) and under better control.

The future collaborator employed under this position will model the electrochemical processes taking place at cathodes using multiscale simulation methods. Initially, the investigation will address the comparison of redox properties for various molecular systems between the homogeneous and the heterogeneous phase at bare metal surfaces. With the progress of the project the same processes will be investigated in the presence of different coating polymers, with the scope of facilitating the design of the best reactive conditions.

It is therefore necessary to set up a simulation framework that allows to study the interaction between cathodic material and a substrate - apart from quantum-chemical calculations of small systems, multiscale approaches will be employed to simulate complex deoxygenation reactions taking into account the electrode and solvent environment.

The work will be conducted in direct collaboration with the experimental group of Prof. Siegfried Valdwogel and the computational physics groups of Prof. Friederike Schmid and Prof. Thomas Speck at JGU, and with the Hylleraas Centre for Quantum Molecular Sciences at the University of Oslo, Norway (UiO). The future collaborator is thus expected to spend some time at UiO for scientific visit and to improve the exchange of ideas with the multiscale modelling group there.

Requirements/qualifications:

- Applicants must hold a PhD or equivalent in Chemistry, Physics, Computer science or similar fields.
- Documented training in either theoretical, computational chemistry, condensed matter theory, molecular physics or close/equivalent topics is required
- Knowledge of quantum mechanics and electronic structure theory is required
- Experience with molecular modelling, and use of ab initio MD codes and enhanced sampling techniques is desired
- Knowledge of statistical mechanics is desired
- Programming skills are desired
- The candidate must have fluent oral and written communication skills in English
- The applicant must be willing to spend periodic visits to collaborators abroad

We offer:

- Salary EUR at least 4.000 € per month depending on qualifications and seniority as PD Research Fellow

How to apply:

The application must include:

- Cover letter. Statement of motivation and research interests
- CV (summarizing education, positions and academic work - scientific publications)
- Copies of educational certificates, transcript of records
- list of publications and academic work that the applicant wishes to be considered by the evaluation committee
- Names and contact details of 2-3 references (name, relation to candidate, e-mail and telephone number)

The application, with attachments, should be sent to to Prof. Jürgen Gauss (email: gauss@uni-mainz.de), Prof. Gregor Diezemann (email: diezemann@uni-mainz.de) or to Prof. Michele Cascella (email: michele.cascella@kjemi.uio.no). The position will remain open until a suitable candidate is found. Applicants are advised to attach an explanation of the grading system of their university. Please note that all documents should be in English or German. Applicants may be called in for an interview.