

Under the auspices of the Center of Electrochemical Sciences (CES) we are looking for a

## Post-Doctoral Researcher

for a joint project between the CMC research group (Dr. Rochus Schmid, Ruhr-University Bochum) and the department for Interface Chemistry and Surface Engineering /Atomistic Modelling Group (Prof. Martin Stratmann/Dr. Alexander Auer, MPIE Düsseldorf).

We are looking for a researcher with Ph.D. from chemistry, chemical engineering, physics or materials sciences or computer science. The candidate should have experience in method development of quantum mechanic codes. She/he should be either fluent in Fortran or preferentially have experience with the combination Python/C, which is the mandatory coding style in the project, and should have experience in parallel programming using MPI message passing. The candidate will work in a small and flexible "team environment" embedded in groups at the Ruhr-University Bochum and Max-Planck-Institute for Iron Research, communicating with the collaboration partners from theoretical and experimental chemistry and physics.

The target of the candidates work will be to modify and extend an existing real space DFT code developed by one of the project partners, towards first principles calculations of electrochemical reactions on charged surfaces and in the presence of an electrolyte.

This involves mainly the computation of the electrostatic problem, which is handled already by a multigrid accelerated Poisson-solver. This way, using purely numeric real space discretized wave functions and densities, atomistic first principles simulations of systems can be carried out that are of high relevance for current energy research on new forms of energy generation and storage, as well as in materials sciences.

Applications will be accepted until the position has been filled.

The Max-Planck society is an equal opportunities employer. Women are strongly encouraged to apply and will be given preference over male applications with a compatible scientific profile. Interested candidates should send their CV including research interests, recent publications and contact data for two references preferably by email to [alexander.auer@mpie.de](mailto:alexander.auer@mpie.de)

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