University of Stuttgart
Germany

Institute for Computational Physics

Director
Prof. Dr. Christian Holm

Institute for Computational Physics, Allmandring 3, 70569 Stuttgart, Germany

Contact
Allmandring 3
70569 Stuttgart • Germany
T +49 711 685-63701
F +49 711 685-63658
e-mail:
holm@icp.uni-stuttgart.de

www.icp.uni-stuttgart.de

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Call for PhD position on atomistic modelling of electrolytes for electrocatalysis of CO2-reduction under confinement

The Institute for Computational Physics at the University of Stuttgart is seeking a highly motivated PhD candidate perform atomistic simulations to study oversolubility and electrolyte properties under confinement and constant potential situations for electrocatalysis of CO2-reduction under confinement. The research should be carried out under the supervision of Prof. Christian Holm in close collaboration with the experimental groups of Prof. Elias Klemm and Dr. Stefan Naumann from the Chemistry Department of the US, Germany within the CRC 1333 (www.crc1333.de).

Background

Electrocatalytic reduction of CO2 plays an important role in using abundant carbon dioxide as a feedstock for chemical reactions. The goal of the current project is to enhance the fundamental knowledge of electrocatalytic reduction of CO2 under confinement by means of all-atom MD simulations under constant potential simulations in combination with experiments. It is also envisaged to construct a theoretical continuum model that should be able to describe the reaction process under consideration. To this a suitable system of partial differential equations will be solved with an existing electrokinetic model.

What we are looking for

Applicants should possess a master degree (or equivalent) in Physics, Physical Chemistry or related areas. A strong background on statistical mechanics and knowledge of all-atom molecular dynamics simulations, as well as willingness for collaborations and team work is expected. The main task consists of carrying out atomistic simulations using the simulation package Lammps (www.lammps.org) to gain fundamental understanding of the CO2 reduction process under applied potentials and in confinement.

Together with available experimental data a theoretical continuum model should be developed and tested. Therefore, a solid background on basic programming (mainly Python and/or C/C++) for code developing and data analysis is advantageous.

What we are offering

- A part-time position in TVL-E13 remuneration of the German State Employees for at least three years, with possibility of extension.
- The opportunity to get to know a broad variety of simulation approaches and techniques.
- Close interaction with other groups on theoretical modelling and experiments.
- An interdisciplinary and flexible research environment where we also encourage the contribution of new research ideas and directions.
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The position is available starting July1, and will be open until the position is filled. Please send your applications as PDF file to application@icp.uni-stuttgart.de, including CV, 2 letters of reference, and a motivation letter.

In an effort to strengthen the presence of female workers in scientific areas, the University of Stuttgart invites women to apply for this job opening. Disabled people will have priority as long as equally qualified.