Computational PhD Positions at Utrecht University:
Atomistic Modeling of Interfaces in Energy Materials with Machine Learning

The Materials Chemistry and Catalysis Group (MCC) at the Debye Institute for Nanomaterials Science (DINS), Utrecht University has immediate openings for computational materials PhD positions for a project related to the modeling of electrochemical energy storage and conversion materials. The PhD students will work under the supervision of Assistant Professor Nongnuch Artrith on projects involving the atomistic modeling of surfaces and interfaces with density-functional theory (DFT) and interatomic potentials to understand and predict the properties of electrochemical devices such as batteries and catalysts. In particular, machine learning-based techniques will be used extensively in this project, including the development of machine-learning potentials [1-7] with our open-source Atomic Energy Network (ænet) package.

The PhD students will interact closely with experimental and theoretical scientists at MCC and DINS.

Applicants should have:

- Background knowledge in first-principles electronic structure theory and
- Experience in scientific programming (experience in GPU is a plus).

Additional experience in one or more of the following areas will be considered an asset:

- Experience with periodic DFT calculations, ideally for surfaces and/or interfaces;
- Materials for electrochemical energy storage/conversion;
- Application of machine learning to materials science; and
- Automated (high-throughput) calculations.

Applications should be submitted online here as PDF files containing all materials to be given consideration. Please include the following files:
- Your letter of motivation;
- Your updated curriculum vitae;
- Copies of your Academic Diplomas (BSc/MSc);
- List of publications (if any);
- The names and contact information of 2 references.

We ask those interested to contact Dr. Artrith (n.artrith@uu.nl) for further details about the positions.

Utrecht University is a friendly and ambitious university at the heart of an ancient city. We love to welcome new scientists to Utrecht --- a thriving cultural hub that is consistently rated as one of the world's happiest cities. We are renowned for our innovative interdisciplinary research and our emphasis on inspirational research and excellent education.

We value diversity in our work environment. Candidates of all genders, ages, races, ethnicities, sexual orientations, and disability statuses are encouraged to apply

[1] N. Artrith and A. Urban, *Comput. Mater. Sci.* **114** (2016) 135-150.
[2] N. Artrith, A. Urban, and G. Ceder, *Phys. Rev. B* **96** (2017) 014112.
[3] N. Artrith, *J. Phys. Energy* **1** (2019) 032002.
[4] A.M. Cooper, J. Kästner, A. Urban, and N. Artrith, *npj Comput. Mater.* **6** (2020) 54.
[5] T. Morawietz and N. Artrith, *J. Comput. Aided Mol. Des.* **35** (2021) 557–586.
[6] A.M. Miksch, T. Morawietz, J. Kästner, A. Urban, and N. Artrith, *MLST.* **2** (2021) 031001.
[7] N. Artrith, K.. Butler, F.X. Coudert, S. Han, O. Isayev, A. Jain, and A. Walsh, *Nat. Chem.* **13** (2021) 505–508.