CSC-RUB PhD Project Proposal

Title: Discovery of new high entropy alloy electrocatalysts

Sector of research: Materials Science/electrochemistry

Degree awarded: PhD

Keywords: Combinatorial Materials Science, high-throughput characterization, high entropy alloys, complex solid solutions

Supervisor of PhD project: Prof. Dr. Alfred Ludwig, e-mail: alfred.ludwig@rub.de

Research focus of supervisor:

My research focus is discovery of new materials using combinatorial synthesis of thin film materials libraries and high-throughput characterization combined with artificial intelligence tools. My international group works on establishing composition-processing-structure-function diagrams for multifunctional materials. I have led many scientific projects which have led to about 300 publications (H index: 41, google scholar). My current research interests are: 1) materials discovery using combinatorial deposition of materials libraries and high-throughput characterization, 2) machine learning in materials science and autonomous experimentation 3) materials for future energy systems, e.g. electrocatalysts.

Publications:

(1) T. A. A. Batchelor, T. Löffler, B. Xiao, O. A. Krysiak, V. Strotkötter, J. K. Pedersen, C. M. Clausen, A. Savan, Y. Li, W. Schuhmann, J. Rossmeisl, **A. Ludwig** (2021) *Complex solid solution electrocatalyst discovery by prediction and high-throughput experimentation*, Angewandte Chemie 60, 6932–6937

(2) B. Xiao, A. Savan, X. Wang, **A. Ludwig** (2021) *Phase constitution of the noble metal thin-film complex solid solution system Ag-Ir-Pd-Pt-Ru in dependence of elemental compositions and annealing temperatures*, Nano Research, https://doi.org/10.1007/s12274-021-3516-7

(3) P. M. Maffettone, L. Banko, P. Cui, Y. Lysogorskiy, M. Little, D. Olds, **A. Ludwig**, A. I. Cooper (2021) *Crystallography companion agent for high-throughput materials discovery*, Nature Computational Science 1, 290 – 297.

(4) **A. Ludwig** (2019) *Discovery of new materials using combinatorial synthesis and high-throughput characterization of thin-film materials libraries combined with computational methods*, npj computational materials 5, 70

(5) T. Löffler, H. Meyer, A. Savan, P. Wilde, A. Garzón Manjón, Y. T. Chen, E. Ventosa, C. Scheu, **A. Ludwig**, W. Schuhmann (2018) *Discovery of a multinary noble metal free oxygen reduction catalyst*, Adv. Energy Mater. 8, 1802269

Summary of research plan

Background: High-entropy alloys (HEAs) have been discovered as a potentially paradigm-changing class of electrocatalysts. Consisting of five or more elements, HEAs provide abundance of active sites, however the challenge is to identify out of millions of possible quinary systems the best ones for different electrochemical applications.

Study objective: The aim is to efficiently identify novel HEAs for electrochemical applications. This will be achieved by depositing thin film materials libraries by combinatorial co-sputtering. These materials libraries will be investigated by high-throughput methods for their compositional, structural and functional properties.

Expected Results: New electrocatalysts with high activity and stability.

Methods: combinatorial magnetron sputter systems and a suite of high-throughput characterization tools

Candidate Requirements:

- an excellent master's degree in materials science
- knowledge in thin films and electrochemistry is appreciated
- a high level of spoken and written English (IELTS band score of 6.5 or higher)

Motivation for CSC application: The successful candidate will be working in one of the leading groups in combinatorial materials science. She or he will have access to a world-class set of unique experimental infrastructure for materials discovery. We provide students with an international and interdisciplinary platform to conduct high-level scientific research.