CSC-RUB PhD Project Proposal

Title: 3-D atomic imaging of catalyst nanoparticles by atom probe tomography

Sector of research: Materials Science/Materials Chemistry

Degree awarded: PhD

Keywords: Atom probe tomography, transmission electron microscope, nanoparticles synthesis and characterisation

Supervisor of PhD project: Tong Li, e-mail: tong.li@rub.de

Research focus of supervisor:

My research focus is to utilize high-end materials characterisation techniques including atom probe tomography and transmission electron microscopy to study structure and chemistry at surfaces, interfaces or in phases of catalyst materials and high-strength alloys. The aim is to establish relationships between synthesis (or processing), structure and performance, thereby providing new insights into materials design. I have led various cross-disciplinary projects which have led to ~50 important publications (H index: 23) in high-quality refereed journals such as Science, Nature Catalysis, Angewandte Chemie and ACS catalysis. My current research interests are: 1) spinel/perovskite nanoparticle synthesis and 2) high-end characterisation and electrochemical measurements of oxide nanoparticles for water splitting, 3) phase transformation in Ti alloys/high entropy alloys.

Publications:

(1) A. BalaKrishnan, N. Blanc, U. Hagemann, P. Gemagami, K. Wonner, K. Tschulik, **T. Li**, *Direct detection of surface species formed on iridium electrocatalysts during the oxygen evolution reaction*, Angewandte Chemie International Edition (2021) doi: 10.1002/anie.202106790

(2) M.J. Lai, **T. Li**, F.K. Yan, J.S. Li, D. Raabe, *Revisiting ω phase embrittlement in metastable β titanium alloys: Role of elemental partitioning*, Scripta Materialia (2021), 193, 38-42

(3) Z. Ji, **T. Li***, OM. Yaghi*, *Sequencing of metals in multivariate metal-organic frameworks*, Science (2020), 369 (6504), 674-680 (*corresponding author)

(4) **T. Li**, M. Lai, A. Kostka, S. Salomon, S.Y. Zhang, C. Somsen, MS. Dargusch, D. Kent, *Composition of the nanosized orthorhombic O' phase and its direct transformation to fine α during ageing in metastable β-Ti alloys*, Scripta Materialia (2019), 170, 183-188

(5) **T. Li**, O. Kasian, S. Cherevko, S. Zhang, S. Geiger, C. Scheu, P. Felfer, D. Raabe, B. Gault, and K. Johann Jakob Mayrhofer. *Atomic-scale insights into surface species of electrocatalysts in three dimensions*. Nature Catalysis (2018), 1, no. 4: 300-305.

Summary of research plan (ca. 300 words):

Background: Development of better electrocatalysts requires a through understanding of the surface composition, structure, and their contribution to the catalytic reactions. However, the effects of the operating environment on the surface composition, structure and stability of electrocatalysts are poorly understood at the atomic-scale. This knowledge will be required to produce the improved catalysts needed for future energy- and materials-efficient technologies. But identifying the chemical nature and 3D location of the individual atoms is a notorious challenge for the conventional surface technique, chemical spectroscopy and electron microscopy.

Study objective: The aims is to synthesis and reveal three-dimensional surface and internal structure and chemistry of catalyst nanoparticles (for oxygen evolution reaction and oxygen reduction reaction), with single atom sensitivity, before and after electrochemical treatment.

Expected Results: New approaches to improve the sample preparation will be developed to enhance the quality of the APT data obtained. The obtained atomic-scale information will be correlated to activity to explore reaction or degradation mechanisms, which will provide a rational guide to nano-engineering catalysts in order to develop cost-effective and high efficiency sustainable energy sources.

Methods: atom probe tomography, transformation electron microscopy, X-ray photoelectron spectroscopy, electrochemical measurements

Candidate Requirements:

- an excellent master degree in materials science, inorganic chemistry, nanoparticle synthesis, or electrochemistry
- experience with synthesis of core-shell alloyed nanoparticles or oxide nanoparticles (e.g. perovskites) for water electrolysis
- can independently conduct potentiostat measurements including cyclic voltammetry, electrochemical impedance spectroscopy, chronopotentiomery, Chronoamperometry etc
- a high level of spoken and written English (IELTS band score of 6.5 or higher)

Motivation for CSC application (max 250 words): The successful candidate will be working in the new research centre for interface-dominated high-performance materials (ZGH) at Ruhr University Bochum, which houses a large and comprehensive suite of equipment dedicated to nanostructure analysis; the centre is among the best facilities of its kind in the world. She or he will have access to a world-class set of laboratories and more than five major microscopy platforms, including the state-of-the-art atom probe, aberration-corrected TEM and focused ion beam. My research group collaborates intensely with international universities and research institutes such as Tsinghua University, University of Oxford and University of Sydney etc. We aim to provide the students with an international and interdisciplinary platform to conduct high-level scientific research.