Redox Exsolution of Metal Nanoparticle Electrocatalysts for Electrochemical Energy Conversion Technologies

Supervisors

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Preferred background of candidate(s)

Preferred background depending on the project:
1. Experimental (MSc or BSc level): Experience with synthesis and sample preparation (e.g., KJM2500, KJM5100, MENA1001), scanning electron microscopy (SEM).

2. Data analysis (MSc level): Familiarity with statistical data analysis methods (e.g. IN1900 , FYS-STK3155, FYS-STK4155, FYS4150, FYS4240) using open-source programming languages, e.g. Python.

3. Computational (MSc level): Experience with Density functional theory (DFT) simulations (FYS-MENA4111)

Number of available projects

2-3

Preferred project period

Start: June 6-12th, or sometime from early July
Main work period: June-August

Outline of project work including expected outcomes/deliverables

Background: Metal nanoparticle catalysts dispersed on the surface of a perovskite oxide support show great promise in solid-state electrochemical devices for energy conversion and electrification of chemical processes involving hydrogen. While nanoparticles typically maximize catalytic activity, they are also prone to agglomeration over time at elevated temperatures. Breakthrough electrocatalyst performance and durability has been achieved by direct growth of nanoparticles from the oxide support by *exsolution* – the exsolved nanoparticles are partly embedded in the oxide, and thus exhibit strong anchoring that inhibits agglomeration (Figure 1).[1,2]

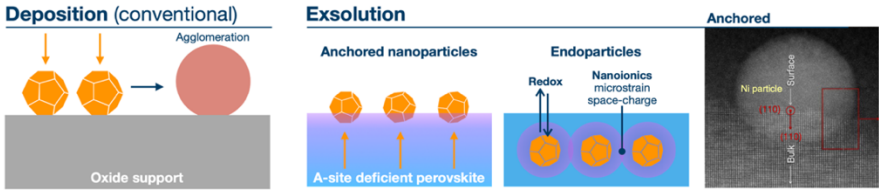

Figure 1: Schematic illustration of deposited metal nanoparticles (orange) that agglomerate (left), anchored nanoparticles and embedded endoparticles formed by exsolution (middle), and TEM cross-section image of anchored Ni nanoparticle.

The student research project work consists of three parts that can be combined in several ways:

1. Experimental: Systematic study of the role of temperature and gas atmosphere on the redox exsolution process. The work will involve synthesis and sintering of transition metal doped $La_{1-x}Sr_xTiO_3$ perovskites with solid-state reaction and annealing of the transition metal loaded samples under controlled temperature and atmosphere. The size and distribution of exsolved metal nanoparticles will then be investigated by SEM.

[1] J. H. Kim, J. K. Kim, J. Liu, A. Curcio, J. S. Jang, I. D. Kim, F. Ciucci, and W. C. Jung, Nanoparticle Ex-Solution for Supported Catalysts: Materials Design, Mechanism and Future Perspectives, *ACS Nano* 15 (2021) 81-110.
[2] D. Neagu, G. Tsekouras, D.N. Miller, H. Ménard, J.T.S. Irvine, In situ growth of nanoparticles through control of non-stoichiometry, *Nat. Chem.* 5 (2013) 916–923.

2. Data analysis: Develop data analysis tools for image processing of SEM images of exsolved metal nanoparticles from the experimental project. The methods will be based on Voronoi diagrams and Hough transforms for detecting and counting grains and exsolved particles. Both methods are available within the SciPy-library, and similar tools are published at multiple open-source Github repositories which will be used for inspiration. The tool will be used for automation of quantitative analysis of the exsolved metal nanoparticles (counting, size and shape) and the porosity of the host material.

3. Computational: Use of DFT to study the transition metal doping of $La_{1-x}Sr_xTiO_3$ perovskites. Transition metals such as Ni, Cu, Fe, Rh, will be introduced in different sites in the lattice. Structural relaxation, stability, and charge state will be studied for the transition metal defects, among other parameters.