About the CRC

The Collaborative Research Centre (CRC) 1625 unites scientists from diverse disciplines and institutions. Our strength lies in the deep collaboration between:

- Materials science
- Surface science
- Electrochemical science
- Theory and Simulation science
- Data science

Our central focus: Surface Atom Arrangements (SAA)

We combine theoretical, experimental, and data-driven methods to achieve atomic-scale control of SAA in Compositionally Complex Solid Solutions (CCSS) and to design surfaces tailored for electrocatalysis on the example of HER.

Next-generation surfaces for future catalysis: CCSS & SAA

We explore CCSS model systems composed of five noble metals forming a single-phase crystal structure. These complex alloys offer promising pathways for sustainable energy conversion, especially in electrocatalysis, where surface properties are key.

We aim to:

- Understand and control of SAA
- Explore how SAA change under different conditions
- Link SAA to electrochemical performance

CRC1625

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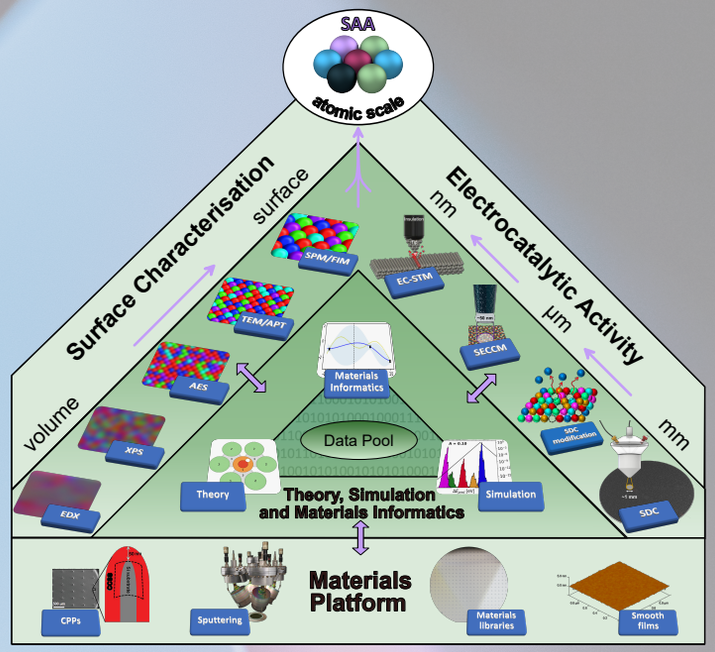
Overview



The CRC aims to understand and control the **atomic-scale surface structure** of CCSS, focusing on the first few atomic layers. Our **scale-bridging** experimental approach, from volume to the surface, is integrated with theory and data science to enable control over SAA. Our **materials platform** provides tailored model systems to systematically explore how volume composition, crystal orientation, defects, and electrochemical conditions influence the surface structure. **Electrocatalytic activity** serves as a functional probe to evaluate and guide SAA design. All **data** are collected in a specifically tailored Research Data Management System (RDMS) and analyzed using materials informatics. This holistic, interdisciplinary strategy enables us rationally design CCSS surfaces for advanced electrochemical applications.

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German Research Foundation

more information

Collaborative Research Centre 1625

Atomic-scale understanding and design of multifunctional compositionally complex solid solution surfaces

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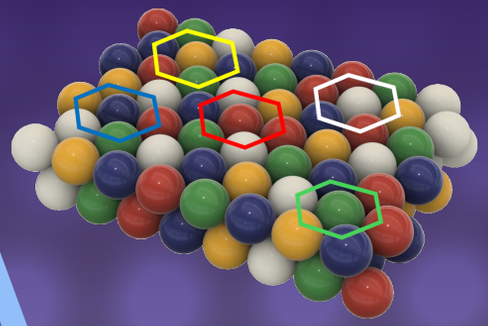
RUHR UNIVERSITÄT BOCHUM RUB

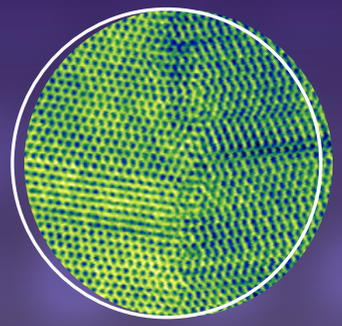
MAX PLANCK INSTITUTE FOR SUSTAINABLE MATERIALS

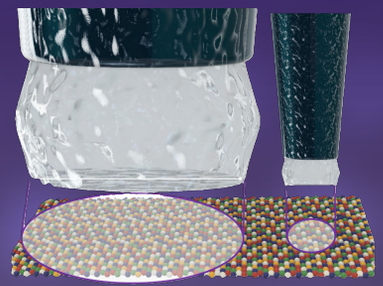
UNIVERSITY OF COPENHAGEN

Technical University of Munich

UNIVERSITÄT DUISBURG ESSEN







A — Theory, simulation, data-guided design and synsthesis of CCSS surfaces

A01 — Theoretical electrochemistry of CCSS surfaces and high-throughput exploration of CCSS thin film systems
A. Ludwig, Ruhr University Bochum
J. Rossmeisl, University Copenhagen

A02 — Microstructure design of quasi-single-crystalline and smooth model thin films
A. Ludwig, Ruhr University Bochum
D. Raabe, Max Planck Institute SusMat

A03 — Simulation of segregation and ordering at CCSS surfaces
R. Drautz, Ruhr-University Bochum

A04 — Ab initio simulations of electrochemical reactions at CCSS surfaces
J. Neugebauer, Max Planck Institute SusMat

A05 — Data-guided experimentation and machine learning
M. Stricker, Ruhr University Bochum

A06 — Establishing a knowledge graph for the design of CCSS surfaces
M. Acosta, Technical University Munich

B — Atomic-scale characterisation of CCSS surfaces

B01 — Accelerated atomic-scale exploration of phase evolution in CCSS systems using combinatorial processing platforms
Y. Li, Ruhr University Bochum

B02 — Revealing the relations between surface atomistic coordination and electrochemical performance of CCSS towards HER
T. Li, Ruhr University Bochum

B03 — High resolution (S)TEM investigation of the surface and other defects in CCSS
C. Scheu, Max Planck Institue SusMat
C. Somsen, Ruhr University Bochum

B04 — Enabling (quasi)-in-situ analytical field-ion microsopy of active CCSS catalysts
B. Gault, Max Planck Institute SusMat
C. Freysoldt, Max Planck Institute SusMat

B05 — Real-space determination of local atomic arrangements of CCSS
K. Morgenstern, Ruhr University Bochum

ECRG — High-Entropy Intermetallics for Electrocatalysis
R. Zerdoumi, Ruhr University Bochum

C — Evaluation of CCSS surfaces using electrochemical tools

C01 — Electrochemical characterisation - High-throughput electrocatalytic screening and single-entity nanoelectrochemistry
W. Schuhmann, Ruhr University Bochum

C02 — Identification of statistically distributed active SAA on a CCSS surface using zooming-in SECCM activity maps
C. Andronescu, University Duisburg Essen

C03 — Elucidating the influences of electrochemically tuned surface composition on the HER at CCSS
K. Tschulik, Ruhr University Bochum

C04 — Identification of electroactive sites at the surface of CCSS under reaction conditions
A. Bandarenka, Technical University Munich

S — General characterisation of thin films and surfaces
J. Pfetzing-Micklich, Ruhr University Bochum

INF — FAIR collection, curation and management of multidimensional research data
M. Stricker, Ruhr University Bochum
V. Dudarev, Ruhr University Bochum