Research Project #1

Modelling Water-Land-Energy Trade-offs and Synergies for Sustainable Energy Transitions (ICE-2 & IBG-3)

Growing pressures on water, land, and energy systems have made their integrated management a central challenge for sustainable development and climate resilience. In regions undergoing rapid demographic growth and energy transitions, such as Sub-Saharan Africa, the interplay between these resources is particularly pronounced. The deployment of renewable technologies often alters land use, affects water availability, and interacts with agricultural or ecological systems in complex ways. Yet, conventional modeling approaches tend to treat such interactions as static constraints rather than dynamic relationships shaped by local context. This has led to models that are robust to highly regulated settings but poorly transferable to areas where environmental governance and land-use negotiations are fluid.

Existing frameworks such as GLAES, developed at ICE-2, provide an excellent open-source basis for assessing spatial suitability and exclusion zones in renewable energy planning. However, such models typically apply binary exclusion logic defining areas as either feasible or not based on static thresholds (e.g., distance to airports, roads, or protected areas). While effective for European contexts with strong regulatory coherence, this approach overlooks the context-dependent trade-offs that characterize project planning in developing economies. For instance, as it is the case of Olkaria geothermal field in Kenya located within a natural reserve and on indigenous land, the coexistence of energy infrastructure, agricultural activity, and protected land often results from local agreements rather than rigid compliance. In such settings, purely rule-based exclusions risk obscuring viable development options and overlooking synergies.

This doctoral project addresses this gap by developing a flexible, spatially explicit modeling framework capable of representing water-land-energy (WLE) interactions through a spectrum of feasibility rather than exclusion. Building on the computational foundation of GLAES, the research aims to introduce graded feasibility layers that quantify trade-offs and co-benefits among resource uses. This approach combines optimization-based system analysis (ICE-2) with biophysical process modeling (IBG-3). The candidate will leverage existing modeling capacities at ICE-2 to represent energy transitions under multi-objective constraints, while drawing on IBG-3's expertise in hydrological modelling, land surface modelling and uncertainty analysis to implement environmental realism into system modeling.

The framework will be tested in a regional case study in Sub-Saharan Africa, Latin America, or comparable regions, chosen for their strong resource interdependencies and frequent negotiation between energy development, agricultural use, and ecological preservation. Using spatial and socio-economic data, the model will evaluate scenarios emphasizing different resource priorities and identify integrated strategies which can deliver maximal co-benefits. This will help informing development pathways that align with the Sustainable Development Goals (SDGs 6, 7, 13, and 15) and support just and context-sensitive transitions. Beyond its analytical innovations, the project reinforces Forschungszentrum Jülich's strategic objectives on sustainable bioeconomy, energy transition, and climate resilience by providing an open-source, transferable modeling instrument.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Climate and Energy Systems - Jülich Systems Analysis (ICE-2), Director: Prof. Dr.-Ing. Jochen Linßen https://www.fz-juelich.de/en/ice/ice-2
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Bio- and Geosciences - Agrosphere (IBG-3), Directors: Prof. Dr. Jan Vanderborght and Prof. Dr. Wulf Amelung https://www.fz-juelich.de/en/ibg/ibg-3

Specific **requirements**	Master's degree in Energy Systems Analysis, Industrial Engineering, Energy Economics, or a related field with good grades. The candidate should demonstrate strong technical modeling skills and an interest in energy-related, economic, and environmental issues in developing economies. Prior experience in energy, hydrological or land surface modeling preferable.
For **project specific** questions please **contact**	**Dr. Amin Lahnaoui**, Christoph Winkler, Prof. Dr. Sandra Venghaus, ICE-2, a.lahnaoui@fz-juelich.de **Prof. Dr. Harrie-Jan Hendricks-Franssen**, IBG-3, h.hendricks-franssen@fz-juelich.de

Research Project #2

Implications of the European transformation pathway to greenhouse gas-neutral energy systems on air quality and human health (ICE-2 & ICE-3)

Following the ambitious goals of the European Green Deal, the European Climate Law enforces climate neutrality of the European Union's member states by the year 2050. By then, the member states are committed to net-zero emissions of Greenhouse Gases (GHG). To achieve this, European economy is facing large transitions in the use and development of technologies and the supply and storage of carbon neutral energy. However, the pathway towards net-zero GHG emissions is not finally agreed upon.

The ETHOS (Energy Transformation patHway Optimization Suite) modeling suite [1] from the Institute of Climate and Energy Systems – Jülich System Analysis (ICE-2) provides tools to analyze cost-optimal transformation pathways of Europe's energy infrastructure on different scales. It is based on assumptions on techno-economic parameters and the transition of different emission sectors (e.g. buildings, traffic, and industry). ETHOS provides information on potential technological changes in the various emission sectors for individual years of the transformation path. Based on these results, corresponding carbon dioxide (CO_2) emissions can be derived. These transformations of the energy system imply not only the reduction of CO_2 emissions but also of the emissions of air pollutants, such as nitrogen dioxide, sulfur dioxide, and particulate matter. Thus, the different pathways to achieving net-zero GHG emissions have implications for air quality and human health in Europe, which are not currently considered by ETHOS. The HITEC project aims at enhancing the applicability of ETHOS to the prediction of air quality under different energy transformation scenarios. The aim is to relate the reduction of CO_2 emissions to emission reductions of air pollutants considering the current knowledge about emission shares, data from technology emission assessments, and existing datasets on emission transformations from environmental agencies and the Coupled Model Intercomparison Project (CMIP). Finally, the project aims to assess potential ways to include air quality-related boundary conditions into the ETHOS optimization procedure.

To evaluate the changes in air quality due to transformations of the energy systems, the chemistry transport model EURAD-IM (EURopean Air pollution Dispersion – Inverse Model; [2]) developed and operationally used by the Institute of Climate and Energy Systems – Troposphere (ICE-3) is utilized to simulate energy transformation scenarios. For all scenarios, air pollutant emissions are calculated for different years towards 2050. For each of these emission datasets, a full year simulation with EURAD-IM is conducted. To assess the sensitivity of air quality to the emission changes, the meteorology of the year 2024 is kept fixed as a reference simulation, for which the most recent actual emission data is available. The air quality assessment is conducted by replacing the actual emissions in 2024 by the reduced emissions from the scenarios. Thus, the direct effect of emission changes on air pollution can be evaluated. Finally, the impact of the different scenarios on human health will be evaluated using data from the Global Burden of Disease database according to previous studies (e.g., [3]).

The project is subdivided into different tasks:

- Evaluation of different suitable pathway scenarios for net-zero emissions by 2050
    - Investigation and adaptation of the underlying assumptions
    - Potential analysis of the combination of assumptions on different technologies
    - Definition and calculation of scenarios using the ETHOS modeling suite
- Estimation of air pollutant emission changes for each pathway scenario
    - Evaluation of CO_2 emissions from different technologies and related changes
    - Evaluation of the emission ratio of CO_2 and air pollutants for existing technologies
    - Evaluation of existing emission scenarios provided by environmental agencies and climate projections (e.g., CMIP)

        - Calculation of emission changes for different pathways based on technologies defined above
- Simulation of air quality for the ensemble of pathway scenarios in Europe
    - Identification of a reference year for simulating current air quality as baseline
    - Setup of modeling framework for the EURAD-IM to simulate the set of emission pathway scenarios defined above
- Evaluation of the implication of energy transformations on air quality and human health
    - Assessment of the air quality in Europe for each scenario
    - Comparison with air quality guideline levels defined by the World Health Organization in 2021
    - Computation and evaluation of changes in mortality due to air pollution for each scenario
    - Discussion of the potential to incorporate air quality-related boundary conditions within the ETHOS module suite

The project is expected to provide new insights into the potential of changing energy systems for air quality and human health. Thus, the project enables to include air quality related issues into climate mitigation considerations, illustrating the co-benefit of long-term climate mitigation actions on short-term air quality improvements. Further, the project reflects the uncertainty incorporated in the pathway calculations by including different potential pathways into the calculation. Here, the emission scenarios of the CMIP assessment are supplemented by a set of ambitious but realistic transformation pathways using a comprehensive approach. Finally, the project aims to bridge the gap between realistic future transformations of the energy systems and health effects due to air quality improvements.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Climate and Energy Systems - Jülich Systems Analysis (ICE-2), Director: Prof. Dr.-Ing. Jochen Linßen https://www.fz-juelich.de/en/ice/ice-2
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Climate and Energy Systems – Troposphere (ICE-3), Director: Prof. Dr. Anke Nölscher https://www.fz-juelich.de/en/ice/ice-3
Specific **requirements**	- Master's degree in physics, meteorology, natural sciences, computer science or related field to energy systems analysis - Programming experiences in python and/or Fortran - Interest in working with complex simulation frameworks - Experience in data analysis - Experience in handling large datasets - Very good communication skills in English
For **project specific** questions please **contact**	Dr. Theresa Klütz, ICE-2, t.kluetz@fz-juelich.de Dr. Philipp Franke, ICE-3, p.franke@fz-juelich.de

[1] Jülicher Systemanalyse, “ETHOS Model Suite.” Nov. 14, 2025. [Online]. Available: https://www.fz-juelich.de/de/ice/ice-2/leistungen/model-services

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Research Project #3

Regional Climate Risk, Carbon Budgets, and Carbon Removal under Uncertainty (ICE-2 & JSC)

Climate change poses not only gradual damage, but also abrupt, non-linear risks that may trigger irreversible shifts in natural and economic systems. Since Nordhaus' pioneering work on integrated assessment models, the economics profession has increasingly incorporated climate change into formal economic analysis [1]. A major insight from the natural sciences is that many ecological systems contain tipping points, where small additional pressures cause the system to move into an alternative, often much less desirable state [2]. Because the precise location of tipping points is uncertain, economic analysis must account for the possibility, rather than the certainty, of catastrophic transitions. This fundamentally alters the structure of the problem: stability may be lost, non-linearities arise in both constraints and damages, and optimal policy becomes sensitive to even small increases in the probability of tipping. Existing models have made important progress by showing how optimal carbon pricing and precautionary saving respond to these risks [3, 4]. However, they typically use highly aggregated representations of energy use and rarely incorporate mechanisms central to current climate policy debates, such as carbon dioxide removal (CDR) options or explicit carbon budget constraints reflecting the temperature targets of the Paris Agreement.

The PhD project will investigate how carbon budgets and CDR options influence optimal policy, economic resilience, and regional transition pathways under tipping uncertainty. Using a dynamic economic framework, where an economy chooses consumption, investment, energy use, and mitigation under a carbon budget and CDR, the project integrates theoretical modeling, numerical methods, and econometric calibration. By linking climate macroeconomics, applied mathematics, and regional economics, it provides both methodological and policy-relevant insights. The project has the scope to:

- Explore alternative functional forms for production, energy composition, and carbon removal
- Examine stochastic tipping risk representations using hazard rates, Value-at-Risk, or Expected Shortfall measures
- Implement and compare numerical solution methods (e.g., Hamilton-Jacobi-Bellman solvers, dynamic programming, or Monte Carlo simulation)
- Extend the model to multiple regional economies with differing technological and policy characteristics

The PhD project will benefit from the expertise of two complementary institutes: Jülich Systems Analysis (ICE-2) and the Jülich Supercomputing Centre (JSC). ICE-2, (specifically, the Spatial Economics Team) provides high expertise in regional energy transition analysis, applied econometrics, and policy-oriented economic modeling. With a strong foundation in empirical methods and regional economic assessment, the group develops tools to evaluate how technological shifts, decarbonization strategies, and climate policies affect economic structures across regions. This expertise ensures that the project remains anchored in real-world data, policy relevance, and the economic dimensions of energy system transformation. JSC (specifically, the group Algorithms, Tools and Methods Labs: Numerical and Statistical Methods) provides high expertise in both theoretical and numerical analysis as well as statistical methods, algorithm development and its implementation, and different high performance computing infrastructure tailored to the new developed solvers.

Combining both economic modeling and theoretical and practical mathematics, algorithm development and implementation in combination with high-performance computing, this project will generate a sound, theoretically founded modeling and analysis framework that integrates empirical regional analysis, policy evaluation, and advanced numerical methods. Together, the project partners provide the full spectrum of skills from data-driven economic interpretation to sophisticated mathematical modeling and implementation of efficient solvers required to deliver a rigorous and policy-relevant assessment of climate risks, carbon budgets, and regional energy transitions.

Work Packages:

WP1: Literature review and conceptual framework (Months 1-6)

- Survey the theoretical and empirical literature on stochastic climate tipping, carbon pricing, and carbon removal
- Define the analytical baseline model and identify data needs for calibration

WP2: Model development, regional extension, and calibration (Months 6-24)

- Formulate an extended dynamic model that incorporates a carbon budget and carbon removal
- Introduce regional differentiation in technology, energy mix, and adaptation capacity

WP3: Numerical implementation (Months 15-30)

- Develop numerical methods to solve the model under uncertainty and explore sensitivity to key parameters
- Calibrate selected scenarios using data for representative economies or world regions

WP4: Scenario and policy analysis (Months 24-36)

- Simulate policy experiments (e.g. tightening carbon budgets, introducing regional cooperation or fragmentation)
- Evaluate impacts on carbon prices, mitigation and removal efforts, and welfare

WP5: Synthesis and dissemination (Months 24-36)

- Integrate findings from previous work packages
- Summarize theoretical findings, discuss implications for climate policy design

Expected results:

- A flexible modeling framework that links stochastic climate risks, carbon budgets, and carbon removal into a coherent economic system
- Quantitative insights into how regional heterogeneity affects optimal carbon pricing and mitigation strategies
- Computational methods applicable to broader classes of stochastic dynamic climate-economy models
- Policy-relevant findings on how carbon budgets and removal options can stabilize economies facing tipping risks

This project helps bridge the gap between theoretical climate macroeconomics and empirical, region-specific policy design. It enables more realistic models that capture both economic behavior and physical climate constraints. For policy, it clarifies how global temperature goals translate into regional economic constraints and investment strategies. For academia, it shows how numerical and econometric methods can be combined to address dynamic uncertainty in climate policy. The interdisciplinary supervision from economics, applied mathematics, and numerical analysis, will equip the PhD student with strong quantitative skills applicable in academia, public policy, and international organizations. It will furthermore strengthen the competence and international scientific visibility of Forschungszentrum Jülich with regard to interdisciplinary climate policy research.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Climate and Energy Systems - Jülich Systems Analysis (ICE-2), Director: Prof. Dr.-Ing. Jochen Linßen https://www.fz-juelich.de/en/ice/ice-2
Partners of the HITEC Project	Forschungszentrum Jülich, Jülich Supercomputing Centre (JSC), Directors: Prof. Dr. Dr. Thomas Lippert and Prof. Dr. Kristel Michielsen https://www.fz-juelich.de/en/jsc
Specific **requirements**	Master's degree in econometrics, economics, applied mathematics, or a related field relevant to theoretical modeling of energy systems and economics Experience with or willingness to apply energy systems assessment and economic policy design, programming, and numerical simulation of economic systems
For **project specific** questions please **contact**	Dr. Imke Rhoden, ICE-2, i.rhoden@fz-juelich.de

[1] Nordhaus, W.D. *A Question of Balance*. Weighing the Options on Global Warming Policies. 2008: Yale University Press. ISBN: 9780300165982. DOI: https://doi.org/10.12987/9780300165982.

[2] Scheffer, M., S. Carpenter, J.A. Foley, C. Folke, and B. Walker. *Catastrophic shifts in ecosystems.* Nature, 2001. **413**(6856): p. 591-596, https://doi.org/10.1038/35098000.

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Research Project #4

Future plant systems and air quality (ICE-3 & IBG-3)

Plants and air composition are closely coupled. Plants remove carbon dioxide from the air, and in turn emit a multitude of volatile organic compounds. These are not only important for attracting pollinators or defending against herbivores - they are also indicators for plant stress. Moreover, gaseous plant emissions are reactive drivers of atmospheric chemistry and precursors to air pollutants. Climate change and environmental stressors such as heatwaves, drought, pests, and pollution are increasingly affecting all ecosystems, including human-made ones like agricultural vegetation and city trees. Such environmental stressors alter the emission amounts and composition of biogenic volatile organic compounds (BVOCs) from the plant systems. BVOCs contribute to ozone and secondary organic aerosol (SOA) formation, which influence both air quality and climate[1].

However, changes in future BVOC emissions and of resulting changes in their feedback on air quality and climate are not well understood[1]. Existing research suffers from fundamental methodological limitations. Laboratory studies have often examined individual stressors only, or studies on multiple stressors excluded soil and root interactions, thus failing to capture comprehensive ecosystem-scale responses. Field studies provide environmental relevance but cannot isolate mechanistic pathways or control confounding variables. This creates a critical "scaling gap" between controlled mechanistic understanding and real-world predictions. Newer studies show that atmospheric stressors such as tropospheric ozone do not only affect the plant directly but also soil microbial communities and thus the entire terrestrial ecosystem[2]. This PhD project aims to investigate how future climate change and stress scenarios impact plant and soil BVOC emissions from agricultural plants and urban tree species, and how these changes affect atmospheric chemistry and ecosystem function.

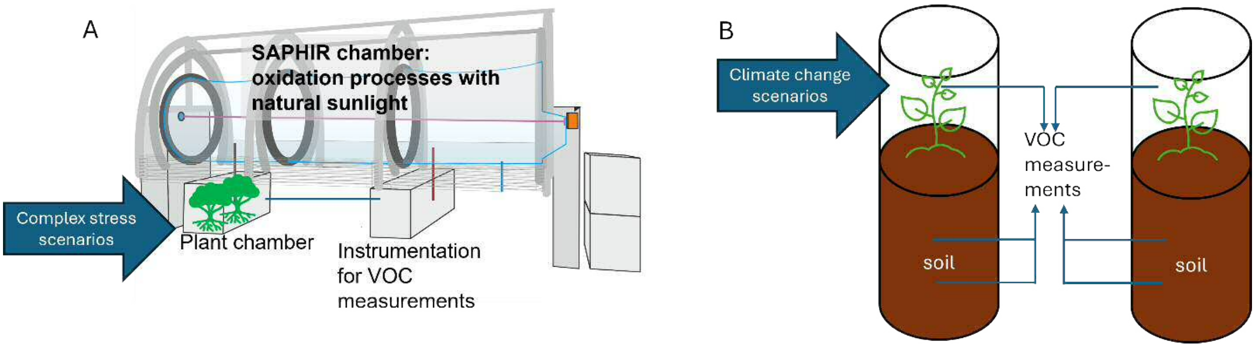

Figure 1. A: SAPHIR-PLUS setup with plant chamber for controlled complex stress experiments with six trees simultaneously and outdoor atmospheric simulation chamber SAPHIR. B: AgraSim setup with six different long-term climate change scenarios that are run in six chambers simultaneously for agricultural crops and their soils.

The candidate will use proton transfer reaction mass spectrometry and gas chromatography to study BVOC emissions in simulation chambers (Agrasim at IBG-3 and the SAPHIR-PLUS chamber at ICE-3) under realistic future climate and stress scenarios. The atmospheric chemistry and aerosol formation impact of the emissions will be investigated using SAPHIR, the atmospheric simulation chamber at ICE-3, and aerosol measurement methods such as aerosol mass spectrometry.

The goal of the project is to establish quantitative relationships between combinations of climate-related and environmental stressors (e.g. temperature, ozone, nutrients) and their impact on biogenic volatile organic compound emissions and atmospheric chemistry to identify biosphere-atmosphere exchange patterns.

Key Tasks in This PhD Project:

- Optimize state-of-the-art mass spectrometry methods (e.g. proton transfer reaction time-of-flight mass spectrometry, aerosol mass spectrometry) and gas chromatography for measuring biogenic volatile organic compounds and their oxidation products
- Conduct experiments to quantify and characterize the emission of volatile organic compounds from relevant plant species and soils under long-term climate change scenarios in the AgraSim facility, and under combined biotic and abiotic stressors in a plant chamber (SAPHIR-PLUS)
- Study photooxidation processes and aerosol formation of characteristic BVOC mixtures under various atmospheric conditions in the large state-of-the-art atmospheric oxidation chamber SAPHIR
- Use advanced data analysis methods including statistical tools on the large multidimensional datasets obtained from the experiments

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Climate and Energy Systems – Troposphere (ICE-3), Supervisors: Dr. Thorsten Hohaus, Jun.-Prof. Dr. Eva Pfannerstill, Director: Prof. Dr. Anke Nölscher https://www.fz-juelich.de/en/ice/ice-3
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Bio- and Geosciences - Agrosphere (IBG-3), Partner: Prof. Nicolas Brüggeman, Directors: Prof. Dr. Jan Vanderborght and Prof. Dr. Wulf Amelung https://www.fz-juelich.de/en/ibg/ibg-3
Specific **requirements**	• M.Sc. in chemistry, physics, meteorology, environmental sciences or a related field • Excellent experimental skills; experience in mass spectrometry or gas-phase measurements is an advantage. • Data analysis experience and/or programming knowledge in Python are an asset • Excellent oral and written communication skills in English • Ability to communicate results clearly in presentations and in writing • Self-motivated, structured working style • Excellent cooperation and teamwork skills
For **project specific** questions please **contact**	Dr. Thorsten Hohaus, ICE-3, t.hohaus@fz-juelich.de Jun.-Prof. Dr. Eva Pfannerstill, ICE-3, e.pfannerstill@fz-juelich.de

[1] Steiner: Role of the Terrestrial Biosphere in Atmospheric Chemistry and Climate, Acc. Chem. Res., 53, 2020.
[2] Agathokleous et al.: Ozone affects plant, insect, and soil microbial communities: A threat to terrestrial ecosystems and biodiversity, Science advances, 6, 2020.

Research Project #5

Influence of multiphase chemistry on tropospheric oxidants in a changing climate (ICE-3 & ICE-4)

In the troposphere ozone (O_3) is an important oxidant, pollutant, and short-lived climate forcer. Yet, despite decades of research global atmospheric models suffer from general overprediction when evaluated against observations [1]. Moreover, the recycling of nitrogen oxides (NO_x) is considered important for correctly predicting past and future O_3 trends [2]. Multiphase chemistry involving production and recycling of radicals and oxidants is extensive and believed to be crucial in the atmosphere. However, global models usually do not account for comprehensive chemistry across phases.

This project aims to unravel the multiphase chemistry with an impact on tropospheric O_3 starting with the quantification of the NO_x-recycling mechanisms. Of particular interest are the global budgets of reactive nitrogen species such as HONO and $ClNO_2$ Their chemistry involves aqueous-phase radical chemistry which in turn can be a driver of O_3 loss. In fact, high radical production in the aqueous phase is fueled by organic compounds and can boost ozone loss [3]. Finally, we will revisit the global budgets of O_3 for the recent past and warmer scenarios [4].

The project will be based on comprehensive observational datasets, such as aircraft missions [5], the TOAR database [6], and TROPOMI satellite retrievals [7]. The datasets will be worked out statistically using new tools as from machine learning. The datasets will be compared to global model simulations including advanced kinetic models for oxidation in the gas-phase, aerosols and cloud droplets [8]. Finally, the impact of future climate change on atmospheric chemistry and pollution will be assessed. Knowledge about these critical mechanisms is a key for assessing the risk of worsening air quality for ecosystem and human health.

Key Tasks in This PhD Project:

- Assess, organize and analyze large observational datasets with respect to ozone and reactive nitrogen species (aircraft, TOAR data base, TROPOMI)
- Develop and include chemical kinetic models in global model framework
- Run various model scenarios (including real world conditions and with a global temperature rise of +2K and +2.75K)
- Evaluate model simulation with observations
- Assess the global impact of including multiphase chemistry on tropospheric O_3 simulations and evaluate the impact of the results

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Climate and Energy Systems – Troposphere (ICE-3), Director: Prof. Dr. Anke Nölscher https://www.fz-juelich.de/en/ice/ice-3
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Climate and Energy Systems – Stratosphere (ICE-4), Director: Prof. Dr. Michaela I. Hegglin https://www.fz-juelich.de/en/ice/ice-4
Specific **requirements**	• M.Sc. in chemistry, physics, meteorology, environmental sciences or a related field • Experience in Earth System Modelling • Data analysis experience and/or programming knowledge • Excellent oral and written communication skills in English • Ability to communicate results clearly in presentations and in writing • Self-motivated, structured working style

	• Excellent cooperation and teamwork skills
For **project specific** questions please **contact**	Dr. Domenico Taraborrelli, ICE-3, d.taraborrelli@fz-juelich.de

[1] P. J. Young, V. Naik, A. M. Fiore, A. Gaudel, J. Guo, M. Y. Lin, J. L. Neu, D. D. Parrish, H. E. Rieder, J. L. Schnell, S. Tilmes, O. Wild, L. Zhang, J. Ziemke, J. Brandt, A. Delcloo, R. M. Doherty, C. Geels, M. I. Hegglin, L. Hu, U. Im, R. Kumar, A. Luhar, L. Murray, D. Plummer, J. Rodriguez, A. Saiz-Lopez, M. G. Schultz, M. T. Woodhouse, G. Zeng; Tropospheric Ozone Assessment Report: Assessment of global-scale model performance for global and regional ozone distributions, variability, and trends. *Elementa: Science of the Anthropocene* 1 January 2018; 6 10. doi: https://doi.org/10.1525/elementa.265

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[7] Heue, K.-P., Loyola, D., Romahn, F., Zimmer, W., Chabrillat, S., Errera, Q., Ziemke, J., and Kramarova, N.: Tropospheric ozone retrieval by a combination of TROPOMI/S5P measurements with BASCOE assimilated data, Atmos. Meas. Tech., 15, 5563–5579, https://doi.org/10.5194/amt-15-5563-2022, 2022.

[8] Rosanka, S., Tost, H., Sander, R., Jöckel, P., Kerkweg, A., and Taraborrelli, D.: How non-equilibrium aerosol chemistry impacts particle acidity: the GMXe AERosol CHEMistry (GMXe–AERCHEM, v1.0) sub-submodel of MESSy, Geosci. Model Dev., 17, 2597–2615, https://doi.org/10.5194/gmd-17-2597-2024, 2024.

Research Project #6

Hydrogen Transparency: Bridging Isotopic Forensics and Next-Generation Energy Solutions (ICE-3 & INW-3)

Hydrogen is a key solution for decarbonizing industry and meeting climate targets, but its environmental impact varies widely depending on the feedstock [1]—such as water, biomass, natural gas, or coal. Ensuring transparency and preventing greenwashing require robust methods to trace and quantify emissions. Advanced analytical techniques, including mass spectrometry and isotopic analysis, provide critical insights into production pathways and associated carbon footprints. Here, we merge techniques from air quality research on tracing and quantifying pollutant sources with the advancement of next-generation, climate-friendly energy carriers, which support the transition toward a resource-efficient, greenhouse gas–neutral industrial landscape. By analyzing the isotopic signatures of organic trace components in methanol, a hydrogen-based fuel, the project will reveal the raw materials and processes underlying its production. The findings will inform the design of a transparent and reliable certification framework for hydrogen and hydrogen-based fuels, enabling the widespread adoption of low-emission hydrogen across industrial and consumer applications.

Tasks of the PhD project are:

- developing and optimizing compound-specific stable carbon isotope measurement methodologies for trace organic compounds in methanol, including chromatographic separation, concentration, and detection
- characterizing isotopic fingerprints of methanol derived from various feedstocks and quantifying raw material contributions. This involves calibrating reference materials against international standards to ensure high-precision, traceable isotope measurements
- Integrating complementary gas chromatographic and mass spectrometric techniques to link molecular-level analyses at ICE-3 with mean compositional characterizations at INW-3
- applying isotopic diagnostics to verify the origin and production methods of methanol, supporting the development of a robust hydrogen-carrier fuel certification scheme

We offer:

- an inspiring, interdisciplinary research environment within an international team
- access to a top-tier scientific setting with state-of-the-art laboratories and technological facilities
- opportunities to present at international conferences
- personalized supervision and mentorship through an excellent supervisor-to-student ratio

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Climate and Energy Systems - Troposphere (ICE-3), Director: Prof. Dr. Anke Nölscher https://www.fz-juelich.de/en/ice/ice-3
Partners of the HITEC Project	Forschungszentrum Jülich, Institute for a Sustainable Hydrogen Economy – Reaction Engineering for Chemical Hydrogen Storage (INW-3), Director: Prof. Dr. Peter Wasserscheid https://www.fz-juelich.de/de/inw/unsere-bereiche/inw-3, https://hch2.de/en/
Specific **requirements**	MSc degree (or equivalent) in chemistry, physics, or atmospheric science with at least a “good” overall grade; strong experimental skills; experience in physical chemistry and/or isotope mass spectrometry is advantageous. Ability to work in international teams and proficiency in spoken and written English are required.
For **project specific** questions please **contact**	Dr. Iulia Gensch, ICE-3, i.gensch@fz-juelich.de

[1] International Energy Agency (2025) Global Hydrogen Review 2025. Paris: IEA. Available at: https://www.iea.org/reports/global-hydrogen-review-2025 (accessed November 10th, 2025)
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Research Project #7

Exploring trace gas-related climate impacts linked to the agricultural biosphere (ICE-4 & IBG-3)

Biogenic emissions of trace gases have a multitude of environmental impacts, including contributions to climate change, air quality, and stratospheric ozone depletion. At the same time, global change is influencing the scale and variability of such emissions. While the major greenhouse gases (GHGs: H_2O, CO_2, CH_4, N_2O) have been studied more intensively in this regard (at least for some plants), many open questions still remain – particularly how GHG fluxes change in a changing climate with more weather extremes (such as longer drought periods, followed by heavy precipitation events (e.g., Zhu et al., 2025). The production of indirect GHGs and ozone-depleting substances (ODSs), the feedback mechanisms they trigger, and their consequential impacts are even less well understood. Gases such as molecular hydrogen (H_2) and carbonyl sulfide (COS) are known to be linked to processes that significantly alter the radiative balance of the atmosphere (e.g., Ocko and Hamburg, 2022; Brühl et al., 2012), while biogenic halogenated species such as CH_3Cl, CH_3Br, or $CHCl_3$ can be transported to the stratosphere where they contribute to the continued depletion of the life-protecting ozone layer (WMO, 2022).

This project aims to combine the expertise of the Institute of Bio- and Geosciences - Agrosphere (IBG-3) and the Institute of Climate and Energy Systems - Stratosphere (ICE-4). IBG-3 has ample expertise in studying plant-soil-atmosphere exchange processes. Of particular relevance here are their measurements of plant, soil and ecosystem fluxes of H_2O, CO_2, CH_4, and N_2O. To maximize the process understanding gained from these ongoing measurements, ICE-4 will be developing and carrying out complementary trace gas measurements, with halogenated species, H_2, and COS, being the most interesting among the range of gases to be considered. This is an opportunity to obtain valuable extra information on soil processes (e.g., via the H_2 soil sink), leaf-based gas exchange (e.g., from COS-CO_2 ratio shifts that can be indicative of plant uptake), or potential future ozone layer impacts (e.g., through chloro-/bromocarbon emission changes). Joint measurement activities are planned at IBG-3-maintained long-term field sites (TERENO/ICOS projects) to determine emissions from a range of plants and soil, as well as their spatial and temporal variability. This will be achieved mainly using balloon- and drone-based sensor packages (e.g., Laube et al., 2025) to be developed as part of this project, as well as the concurrent adaptation and optimization of existing measurement systems at both institutes.

In addition, IBG-3 operates the world-class facility AgraSim (https://www.fz-juelich.de/en/ibg/ibg-3/expertise/research-platforms/agrasim) which contains six parallel plant mesocosms that allow to simulate different climate “storylines” under controlled conditions. The project will explore possibilities to use the developed measurement and sampling systems within these mesocosms to determine hitherto unknown potential changes and feedback mechanisms that might impact future climate change and/or agriculture.

The measurements and process understanding generated in this project will ultimately provide valuable information for better quantification of the impact of weather extremes on the trace gas exchange of agricultural ecosystems with the atmosphere.

Key objectives of the proposed PhD project:

- Developing balloon- and drone-based sensor packages primarily focused on the collection of air samples
- Carrying out multiple flights during different seasons with these packages
- Retrieving atmospheric mole fractions, predominantly via lab-based sample analysis techniques, and deriving emission estimates of the trace species
- Quantifying the impact of longer drought periods with subsequent rewetting on soil and ecosystem GHG and other trace gas fluxes
- Extensive comparisons with ongoing long-term measurements of trace species

Tasks to be completed:

- Designing and testing the new airborne packages between late 2026 and late 2027
- Concurrent optimization of the related measurement instrumentation (GC-MS, GC-PDD, optical spectroscopy techniques)
- Flying the new packages predominantly in 2027 and 2028, including subsequent measurements as well as further miniaturization and potential adjustment of the range of target species
- Conducting campaign-based chamber measurements of GHGs and other trace gases during natural drought and rewetting periods
- Comparing the results with those from related previous studies including model-based approaches
- Scientific data interpretation and publication of the findings

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Climate and Energy Systems – Stratosphere (ICE-4), Director: Prof. Dr. Michaela I. Hegglin https://www.fz-juelich.de/en/ice/ice-4
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Bio- and Geosciences - Agrosphere (IBG-3), Directors: Prof. Dr. Jan Vanderborght and Prof. Dr. Wulf Amelung https://www.fz-juelich.de/en/ibg/ibg-3
Specific **requirements**	M.Sc. degree or equivalent in Atmospheric Sciences, Biogeochemistry, Physics, Chemistry or a related field; some experience in meteorology or analytical chemistry would be beneficial
For **project specific** questions please **contact**	Dr. Johannes C. Laube, ICE-4, j.laube@fz-juelich.de Prof. Dr. Nicolas Brüggemann, IBG-3, n.brueggemann@fz-juelich.de

[1] Brühl, C., Lelieveld, J., Crutzen, P. J., and Tost, H.: The role of carbonyl sulphide as a source of stratospheric sulphate aerosol and its impact on climate, Atmos. Chem. Phys., 12, 1239–1253, https://doi.org/10.5194/acp-12-1239-2012, 2012.

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[5] Zhu, G. et al.: Nitrous oxide sources, mechanisms and mitigation. Nat. Rev. Earth Environ. 6, 574–592, https://doi.org/10.1038/s43017-025-00707-5, 2025.

Research Project #8

Designing SOFC Electrodes via Correlative *In-Situ* TEM and 3D Atom Probe Tomography (IET-1 & ER-C-2)

The solid oxide fuel cell (SOFC), which promises the highest efficiency of all fuel cell types, and synergistically related solid oxide (co)electrolysis cell (SOEC) are thought to be the pillars for paving the path towards net carbon zero society. Currently though, the durability of electrodes during long-term operation limits the cycle life of these cells. At the Institute of Energy Technologies - Fundamental Electrochemistry (IET-1), we are working with this topic for many years and have developed industrially promising ceramic-based electrode materials for this purpose **[1,2]**. However, further material engineering is necessary to ensure long-term catalyst activity before these electrodes can be integrated into a commercial system.

Building upon the success of the recent HiTEC project (2022-2025) that established our *in-situ* TEM framework and led to new insights into 2D catalyst exsolution dynamics **[3,4]**, this project will take the crucial next step. This project for the first time would combine two state-of-the-art non-trivial techniques for the SOFC materials, creating a unique, closed-loop feedback system for materials development. Utilizing the newly developed *in-situ* gas-heating-biasing workflow at relevant atmospheric pressure, we will be directly observing catalyst exsolution, activation, and degradation during electrochemical processes. Following the *in-situ* experiment, we will then transfer this same sample to the new TEM-APT (TOMO) **[5]** microscope at Ernst Ruska Centre for Microscopy and Electron Spectroscopy - Materials Science and Engineering (ER-C-2) to conduct a 3D atomic-scale dissection. This will provide the first-ever 3D atomic maps of element distribution at the exsolved catalyst/ matrix interfaces after they have been observed functioning in real-time. These insights will provide the "ground truth" feed back to our materials synthesis group for synthesis of next-generation, degradation-resistant materials.

This project is the ideal bridge between the materials-science mission of IET-1 and the world-class microscopy capabilities of ER-C-2. As the lead institute and HITEC member, IET-1 will be the hub for *in-situ* science, electrochemistry, and materials synthesis. Its responsibilities will include: leading the project and defining the key scientific questions; leading the *in-situ* (gas-heating-biasing) TEM experiments and the FIB-SEM sample preparation; working with its internal "Solid-State Electrolysis & Fuel Cells" focus group to perform all macro-scale electrochemical testing (button cells, EIS) to validate device-level performance; to design and driving the final nano-to-macro correlation and produce new generations of exsolving perovskites. Our cooperation partner, ER-C-2, provides the unique, indispensable infrastructure and expertise for the final atomic-scale analysis. It will be responsible for: providing expert consultation for the APT-specific sample preparation workflow, ensuring high-quality data from the TOMO microscope; executing the novel correlative TEM-APT (TOMO) experiments on the *in-situ* TEM samples; leading the 3D atomic data reconstruction and analysis from the APT; and providing access to and support for its world-class microscopy infrastructure.

For this purpose, the following tasks will be addressed during the three years tenure of the Ph.D.

WP1: Lead *in-situ* gas-heat-biasing TEM experiments - test the degradation hypothesis by tracking dynamic changes in electrode activation, catalyst exsolution, and degradation under electrochemical load.

WP2: Develop and execute a robust FIB-SEM workflow to prepare APT needles from the *in-situ* TEM samples. Execute transfer of the *post-in-situ* sample to the TOMO microscope for correlative 3D Atom Probe Tomography.

WP3: Perform TEM and APT investigation from relevant macro-scale samples. Correlate *in-situ* and macro-scale results to establish a quantitative structure-property-degradation relationship, creating a "materials feedback loop" to inform the design of new materials.

Thus, while working in a highly multidisciplinary, multicultural spirited team at the end of the Ph.D., the candidate will not only master the specific skillsets required to operate advanced TEMs, or design *in-situ* TEM experiments, but also gain in-depth knowledge of industrially relevant SOFC/SOEC processes.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Technologies - Fundamental Electrochemistry (IET-1), Director: Prof. Dr. Rüdiger- A. Eichel https://www.fz-juelich.de/en/iet/iet-1
Partners of the HITEC Project	Forschungszentrum Jülich, Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons - Materials Science and Technology (ER-C-2), Director: Prof. Dr. Joachim Mayer https://www.fz-juelich.de/en/er-c/er-c-2
Specific **requirements**	M.Sc. degree in Materials Science/Physics/Chemistry/ Mechanical Engineering; in-depth understanding of material characterization
For **project specific** questions please **contact**	Dr. Shibabrata Basak, IET-1, s.basak@fz-juelich.de

[1] F. Kunz et al., ECS Transactions, 2023, 111 (6),1667, DOI 10.1149/11106.1667ecst
[2] S.E. Wolf et al., Electrochemistry Communications, 2024, 16, 107799, DOI: 10.1016/j.elecom.2024.107799
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[4] S.E. Wolf et al., Journal of Materials Chemistry A, 2025, 13, 34565-34584, DOI: 10.1039/D5TA04819B
[5] A. Vayyala et al., Microscopy and Microanalysis, 2024, DOI: 10.1093/mam/ozae044.039

Research Project #9

High-throughput material screening and device characterization for the production of green hydrogen using direct PV coupling (IET-1 & IMD-3)

“Green hydrogen” produced electrolytically using renewable resources is central to de-fossilize high carbon-emitting sectors like the transportation sector, but also heavy industries such as steel production and the chemical industry including ammonia synthesis. While electrolyzers have reached relative market maturity for several of the available technologies, many questions regarding their operational stability under dynamic power profiles still exist [1]. This is particularly relevant for the use with only intermittently available renewable energy sources such as photovoltaics (PV), which require long-term storage solutions to compensate for the significant seasonal variations in generation.

One especially attractive operational scenario is the direct coupling of the renewable energy device with the electrolyzer cell. In comparison to a typical grid connection of the electrolyzer cell, this can lead to significant cost reductions for balance-of-plant expenses such as transformers and rectifiers [2]. Additionally, direct coupling to PV enables capturing of excess PV generating capacity at the point of generation, which minimizes the need for grid extensions in future scenarios of massive PV capacity growth worldwide, and particularly in Germany. First studies in cooperation between IET-1 and IMD-3 have shown that an approach using virtual coupling with realistic simulated solar profiles is feasible for long-term operation of over 3000h in PEM electrolysis with comparatively low efficiency loss using commercial materials. There remains however a significant potential for optimization on the path towards highly efficient and stable directly coupled PV-electrolyzer devices [3].

This project aims to build upon these initial results by applying high-throughput approaches both on the fundamental material side as well as on the operational device side. First, a high-throughput characterization platform (HTCP) for rapid material screening is used to find the promising electrocatalysts as candidates for later use in the electrolyzer. The HTCP’s parallel synthesis and rapid electrochemical evaluation are aggregated into three core stages: automated, robotized material library preparation; automated electrochemical characterization to determine the catalyst activity and short-term stability; and parallel, multichannel product selectivity analysis. This creates a unique opportunity to couple experimental data with predictive machine learning algorithms and explore an enormous landscape of material combinations of critical raw material (CRM) free electrocatalysts in an unprecedentedly short time, far surpassing traditional trial-and-error methods.

After suitable candidates are identified, they need to be applied in full electrolyzer cells for durability and performance tests using realistic solar profiles, as there are typically significant gaps between model systems and real cells using membrane electrode assemblies (MEAs) [4]. Furthermore, in real operation not only does the choice of catalyst play a role, but many other parameters (temperature, pressure, flow rate, type of membrane, diffusion/transport layers, etc.) influence the operation, necessitating again the use of rapid screening of different compositions. For this, the available high-throughput electrolysis unit at IET-1 can be used to screen up to 16 electrolyzer cells in parallel. This way relevant electrode parameters such as catalyst loading, in-plane resistance, ionomer content and porosity can be systematically tuned and rapidly tested.

For this project the focus is on PEM electrolysis as it is the most suitable and mature technology for dynamic electrolyzer operation. One of the biggest drawbacks of this technology is the use of noble metals, mainly Pt and Ir, as catalysts. In order to minimize the use of such CRMs the project will focus on the one hand on reducing the amount used through for example suitable support materials and on the other hand, on exploring catalyst combinations with reduced or even no noble metal content such as for example sulfide or phosphide materials for HER (e.g. CoP, FeS_2, MoS_2, etc.), (mixed) metal oxides (e.g. MnO_2, Co_3O_4, etc.) for OER as well as materials doped with low amounts of noble metal or alloy materials .

All in all, the project will aim to develop novel suitable catalyst materials for dynamically operated (PEM) electrolyzers, specifically for direct coupling with solar devices. Ideally this would provide the groundwork for the development of novel highly efficient directly coupled PV-electrolyzer devices that could overcome the significant challenge of seasonality in PV generation as PV capacity is set to exceed grid power capabilities.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Technologies - Fundamental Electrochemistry (IET-1), Director: Prof. Dr. Rüdiger- A. Eichel https://www.fz-juelich.de/en/iet/iet-1
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Energy Materials and Devices - Photovoltaics (IMD-3), Director: Prof. Dr. Christoph Brabec https://www.fz-juelich.de/en/imd/imd-3
Specific **requirements**	M.Sc. degree in Materials Science, Physics, Chemistry, Process Engineering or Mechanical Engineering; experience in electrolyzers or fuel cells preferable
For **project specific** questions please **contact**	Dr. André Karl, IET-1, a.karl@fz-juelich.de Dr. Oleksandr Astakhov, Dr. Tsvetelina Merdzhanova, IMD-3, t.merdzhanova@fz-juelich.de

[1] Alia SM, Stariha S, Borup RL. Electrolyzer Durability at Low Catalyst Loading and with Dynamic Operation. J Electrochem Soc 2019;166:F1164–72. https://doi.org/10.1149/2.0231915jes.

[2] Niederhofer S, Rennhofer M, Hofmann R, Kubicek B, Neussl V. System efficiency analysis of direct coupled PV – PEM electrolyzer systems. Int J Hydrogen Energy 2025;185:151860. https://doi.org/10.1016/j.ijhydene.2025.151860.

[3] Chibuko U, Merdzhanova T, Agbo S, Rau U, Wurstbauer U, Astakhov O. International Journal of Hydrogen Energy Breaking limits of solar-to-hydrogen efficiency via synergy with batteries. Int J Hydrogen Energy 2025;127:38–50. https://doi.org/10.1016/j.ijhydene.2025.04.166.

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Research Project #10

Engineering CO_2 Electroreduction to Value-Added Products with Tailored Anion Exchange Membranes (IET-1 & PGI-6)

Motivation and State of the Art

The electrochemical reduction of CO_2 (eCO_2R) is a promising technology for producing value-added products (e.g., carbon monoxide, formic acid, methanol, ethanol, ethylene) required for a circular, renewable-based economy, while simultaneously mitigating further CO_2 emissions by converting the most significant anthropogenic greenhouse gas into a valuable feedstock. To improve energy efficiency and selectivity toward the target product, technological improvements in key components, such as electrodes, catalysts, cells, and membranes, are fundamental. Anion exchange membranes (AEMs) are of special importance in the eCO_2R by enabling operation in alkaline media, allowing the use of non-precious metal catalysts, and suppressing the competing hydrogen evolution reaction (HER).[1] However, the variety of AEMs remains limited, as their development is largely controlled by industrial companies, where limited knowledge sharing slows innovation in membrane research. ***This project focuses on synthesizing new polymers for dual applications: As ionomers in gas diffusion electrodes and as AEMs in the eCO_2R to carbon monoxide.***

Key research goals for the project

WP1: *Identify and synthesize monomeric scaffolds.*
Based on existing studies on the alkaline stability of cationic groups (e.g., Marino & Kreuer[2]), suitable monomer structures will be identified and partially synthesized. The focus will be on potential ionic conductivity and chemical stability.

WP2: *Polymerization of monomeric units.*
The identified monomers will be polymerized and optimized with respect to functionalization and molecular weight distribution, as molecular weight strongly influences the stability.[3]

WP3: *Membrane and GDE fabrication.*
Membranes and GDEs will be produced from the developed polymers using appropriate techniques (e.g., casting, spray coating). Parameters such as thickness and homogeneity (membrane), catalyst loading, and ionomer content (GDE) will be optimized.

WP4: *Application of fabricated gas diffusion electrodes and AEMs in the eCO_2R to carbon monoxide: Evaluation of key performance indicators.*
The fabricated GDEs and AEMs will be tested in dedicated setups to evaluate their performance (e.g., Faradaic efficiency, cell voltage, energy efficiency).

WP5: *Analysis of structure-performance correlation.*
The developed membranes will be analyzed using structural characterization methods (e.g., AFM, SEM, TEM, SAXS). The aim is to identify structural features (microphase separation, ion density, morphology) that contribute to high electrochemical performance. Both pristine and post-test membranes will be examined to determine possible degradation effects.

Gaining expertise and career prospects via the project

The proposed project will benefit from the synergy of two institutes within Forschungszentrum Jülich working on a project that builds expertise in organic and inorganic synthesis, polymer chemistry, electrochemistry, and material chemistry. PGI-6 brings its expertise in inorganic/organic synthesis, which is essential for WPs 1–2. IET-1 provides its expertise in electrochemistry and material chemistry for WPs 3–5. At IET-1, the research activities are further strengthened by hands-on experience in membrane fabrication and scaling, gained through direct involvement in industrial environments. The established and successful collaboration between PGI-6 (Prof. Kögerler's group) and IET-1 highlights the effective synergy between both institutes. Prof. Kögerler, also serving as a group leader in RWTH Aachen (Institute of Inorganic Chemistry), will make available additional advanced instrumentation required for the project. Regular interaction between PGI-6 and IET-1 will expose the applicant to different methodologies, such as advanced spectroscopic and electrochemical characterization techniques, as well as membrane fabrication and upscaling strategies rooted in industrial practice. This interdisciplinary framework not only ensures high scientific output and publications in leading journals but also equips the applicant with the practical and strategic skills required to bridge academic research and industrial innovation in the field of electrochemical technologies.

Expected Outcomes & Impact

The anticipated outcome is a high-performance, long-term stable AEM specifically engineered for CO_2 to CO electrolysis. Furthermore, by combining molecular-level materials design with application-driven electrochemical validation, design guidelines will be developed. These guidelines will accelerate the development of next-generation membranes applicable to CO_2 electrolysis.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Technologies - Fundamental Electrochemistry (IET-1), Director: Prof. Dr. Rüdiger- A. Eichel https://www.fz-juelich.de/en/iet/iet-1
Partners of the HITEC Project	Forschungszentrum Jülich, Peter Grünberg Institute – Electronic Properties (PGI-6), Director: Prof. Dr. Claus Michael Schneider, Partner: Prof. Dr. Paul Kögerler (https://www.koegerler.ac.rwth-aachen.de) https://www.fz-juelich.de/en/pgi/pgi-6
Specific **requirements**	Master's degree in chemistry, materials science, chemical engineering, or related field. Fluency in English is required; German proficiency is desirable.
For **project-specific** questions, please **contact**	Sven Sören Hartmann, IET-1, s.hartmann@fz-juelich.de Dr. Sergio Calvo, IET-1, s.calvo@fz-juelich.de

(1) Lin, J.; Zhang, Y.; Xu, P.; Chen, L. CO2 electrolysis: Advances and challenges in electrocatalyst engineering and reactor design. *Materials Reports: Energy* **2023**, *3* (2), 100194.
(2) Marino, M.; Kreuer, K. Alkaline stability of quaternary ammonium cations for alkaline fuel cell membranes and ionic liquids. *ChemSusChem* **2015**, *8* (3), 513–523.
(3) Hartmann, S. S.; Schalenbach, M.; Schestakow, M.; Eichel, R.-A. The effect of ionomer molecular weight on gravimetric water uptake, hydrogen permeability, ionic conductivity and degradation behavior of anion exchange membranes. *International Journal of Hydrogen Energy* **2025**, *151*, 150126.

Research Project #11

Oxygen Evolution and Dissolution Mechanisms on IrO_2 and RuO_2 Model Electrodes (IET-2, IET-3 & IET-4)

Context: Green hydrogen production via water electrolysis is essential for storing surplus renewable energy. Among available technologies, proton exchange membrane water electrolysis (PEMWE) is considered the most suitable. However, its reliance on Ir-based catalysts for the oxygen evolution reaction (OER) makes the technology prohibitively expensive. Current state-of-the-art catalysts suffer from dissolution, requiring high loadings of iridium and other PGMs (platinum-group metals) to slow down degradation. To reduce costs, catalyst loadings must be lowered without sacrificing performance, which demands materials that are both more active and more stable. Achieving this is challenging because activity and stability are often negatively correlated [1]. It has been proposed that OER and Ir dissolution share common intermediates: the OER pathway destabilizes the catalyst through formation and cleavage of metal–oxygen bonds, involving both adsorbates and lattice oxygen [2]. Stabilizing these bonds could enhance durability, but according to the Sabatier principle, overly strong binding may reduce OER activity, an argument that holds only if the reaction mechanism remains unchanged. Recent theoretical studies indicate that fundamental differences in OER mechanisms can explain the distinct activity and stability properties among PGM-oxide catalysts [3], and surface defects can introduce additional mechanistic pathways [4]. Moreover, distinct crystallographic orientations of IrO_2 and RuO_2 were found to exhibit different OER activities [5]. Despite these observations, the structure–performance relationships governing OER activity and stability on IrO_2 and other PGM-oxide catalysts remain poorly understood.

Aims: The overall goal of this project is to establish a mechanistic framework that explains both the OER and catalyst dissolution pathways on well-defined oxide model electrodes with controlled structure, morphology, and composition. This framework will guide the rational design of advanced electrocatalysts that simultaneously achieve high activity and high stability, ultimately enabling the replacement of Ir with more abundant and cost-effective elements such as Ru or even non-noble metals.

State of the art: Given its industrial relevance, the OER on Ir oxide electrodes has been intensively studied for decades. A major milestone was the experimental detection of IrO_3, proposed as a key intermediate in both OER and Ir dissolution [6]. This finding enabled refinement of existing mechanistic pathways and helped rationalize structural effects in the OER, such as differences between amorphous and crystalline Ir oxides. However, these insights were largely derived from ill-defined electrodes, which limit atomistic interpretation. A deeper mechanistic understanding can be achieved using single-crystalline electrodes, as demonstrated for Pt. There, the combination of experimental data on surface oxidation and dissolution with density functional theory (DFT) calculations of phase stability led to a comprehensive model explaining Pt dissolution during initial oxidation and during partial reduction of bulk-like oxides [7]. Extending this approach to Ir and Ru oxides is more challenging due to the scarcity of high-quality single-crystal IrO_2 and RuO_2. Recent advances in molecular beam epitaxy (MBE) and pulsed laser or arc plasma deposition have now enabled the fabrication of such model electrodes for electrochemical applications [5, 8]. Preliminary studies have already shown that OER activity depends strongly on the surface structure. However, dissolution was assessed only ex situ, revealing no clear trends in stability. While these initial findings reveal differences in activity and stability, they do not provide the mechanistic insight needed to explain them. Without this understanding, rational design of improved catalysts remains challenging.

Work plan: This collaborative project combines expertise available at different research units of the Research Center Jülich (FZJ), i.e., in experimental OER and catalyst stability (IET-2), vibrational spectroscopy at catalytic surfaces (IET-4), and theoretical electrocatalysis (IET-3) to develop a mechanistic framework for OER and catalyst dissolution. A PhD student will be hired to set up and validate the experimental work at IET-2, while spectroscopic and theoretical studies will be supported through collaboration with IET-4 and IET-3. Well-defined IrO_2 and RuO_2 facets, initially (001) and (110) and later other orientations, will be prepared by Prof. Holtz's group using the recently established MBE method [8].

The OER activity and dissolution kinetics will be measured using online ICP-MS. Only minor modifications to the setup will be required to increase the Ir detection limit, achieved by minimizing the electrolyte-to-electrode-area ratio. The small electrode area enables high-throughput screening, allowing rapid accumulation of a large dataset for further theoretical analysis. The project will systematically explore the effects of electrode potential, time, temperature, and pH on OER and Ir/Ru dissolution. Electrodes exhibiting extreme performance metrics will be selected for detailed mechanistic studies using *in situ* IR and Raman spectroscopy combined with X-ray photoelectron spectroscopy (XPS). In parallel, DFT calculations will be employed to model surface phases, reaction intermediates, and dissolution pathways, integrating experimental and theoretical insights into a unified framework. The framework will guide the design, preparation, and testing of model electrodes with enhanced functionality. The focus will be on replacing Ir with Ru and on improving surface stability through strategies such as surface modification and doping with Ti, Nb, or Ta.

Outcomes: The overall outcome of this project will be the establishment of a comprehensive experimental-theoretical framework for understanding the activity and stability of OER electrocatalysts for PEMWE. This framework will include improvements in the online ICP-MS setup aimed at lowering detection limits, the development of systematic experimental testing procedures considering variables such as potential, time, temperature, and pH, and the integration of spectroscopy with theoretical modeling to gain deeper insights into the coupled mechanisms and intermediates of OER and catalyst corrosion processes. Application of this framework to a variety of materials will enable a better understanding of structure–activity–stability relationships in OER electrocatalysis and support the development of active and stable catalysts with minimal or no Ir content, thereby reducing the cost of green hydrogen production. The PhD student will receive in-depth training and supervision in a network of dedicated experts in experimental and theoretical electrocatalysis, strengthening the collaboration between different FZJ units and the exchange in a vivid group of fellow PhD students. Results of this project will be disseminated through scholarly journals and conference presentations.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Technologies - Helmholtz-Institute **Erlangen-Nürnberg** for Renewable Energy (IET-2 / HI ERN), Director: Prof. Dr. Karl Mayrhofer https://www.hi-ern.de/en
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Energy Technologies - Theory and Computation of Energy Materials (IET-3), Director: Prof. Dr. Michael Eikerling https://www.fz-juelich.de/en/iet/iet-3 Forschungszentrum Jülich, Institute of Energy Technologies - Electrochemical Process Engineering (IET-4), Director: Prof. Dr. Ralf Peters https://www.fz-juelich.de/en/iet/iet-4
Specific **requirements**	M.Sc. in Chemistry, Physics, Material Science, or equivalent. Good knowledge of physical chemistry and surface science.
For **project specific** questions please **contact**	Dr. Serhiy Cherevko, IET-2, s.cherevko@fz-juelich.de Dr. Tobias Binninger, IET-3, t.binninger@fz-juelich.de Dr. Christian Rodenbücher, IET-4, c.rodenbuecher@fz-juelich.de

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Research Project #12

Conformal wet-coating of perovskite on random pyramid texture by controlling the perovskite crystallization process (IET-2 & IMD-3)

Perovskite–silicon tandem solar cells are attracting intense interest because they surpass the efficiency limits of conventional silicon photovoltaics. By combining a wide-bandgap perovskite top cell with a silicon bottom cell, tandems harvest a greater portion of the solar spectrum and have already achieved record efficiencies that surpass those of single-junction silicon. Their compatibility with low-cost, low-temperature processing makes them a practical route to higher-performing, scalable solar modules. Continued work is essential to improve stability and large-area integration so these laboratory breakthroughs can translate into durable, commercially viable clean-energy technologies.

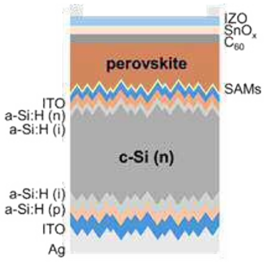

Figure 1: Schematic view of a silicon - perovskite tandem solar cell.

At present, several technologies exist for depositing perovskite layers onto randomly textured silicon pyramids. The most used approach is a hybrid process, in which the inorganic component of the perovskite is first deposited by evaporation, followed by a wet-chemical deposition of the organic component, allowing the two to react and form the perovskite crystal. An alternative method is one-step co-evaporation of all precursors, or sequential evaporation of the inorganic and then the organic species. These vacuum-based routes are used instead of the simpler one-step or two-step solution processes because wet-processed perovskite films typically fail to achieve conformal coverage on micrometer-scale random pyramids. For pyramid textures with heights of about 2–3 µm, the perovskite layer often fails to fully cover the pyramid tips. Increasing the perovskite thickness could, in principle, solve this, but it would result in excessively thick layers at the pyramid valleys, which is detrimental to device performance.

If conformal coating could be achieved using low-cost wet processing, this would be far more attractive than vacuum-based technologies. However, conformality requires that crystallization begins homogeneously across the entire textured surface, independent of whether the location is at the valley or the tip of a pyramid. Achieving these demands requires precise control over heterogeneous nucleation and very rapid, uniform seed formation. Ultimately, this challenge leads back to a deeper understanding of how perovskite crystallization is influenced by substrate morphology, surface energy, and quenching conditions.

The PhD project aims to uncover the crystallization mechanisms of perovskites as a function of texture geometry, surface properties, and processing methods, and to develop a roadmap for engineering truly conformal, wet-processed coatings. This will be demonstrated on high-efficiency perovskite silicon tandem solar cells. This work will combine computational and experimental approaches, and the candidate is expected to spend approximately 50% of their time in Nuremberg at IET-2 and 50% of their time in Jülich at IMD3.

IET-2 will provide the computational infrastructure necessary, including a mesoscale phase field simulation framework that allows for the simulation of crystallization processes in drying solutions deposited on textured surfaces, as well as access to a state-of-the-art high-performance computing infrastructure. The simulations allow for investigation of a wide spectrum of material- and process parameters on the impact of substrate texture, wetting properties, drying, and crystallization kinetics on the perovskite film morphology.

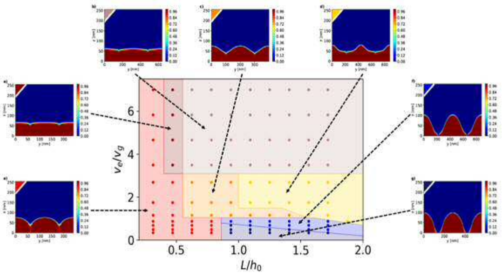

Figure 2: Example of phase field simulations: Morphology of crystals grown in a drying film, depending on the ratio between evaporation rate and growth rate v_e/v_g and on nucleus density L/h_0.

IMD3 will provide the full experimental infrastructure necessary, including the capability to fabricate different texture morphologies, use various TCO and SAM materials, and apply tailored surface treatments that modify surface energy prior to perovskite deposition. IMD3 can also fabricate complete perovskite–silicon tandem devices, with the current reference efficiency reaching 33.4%. With successful conformal coating, the targeted efficiency exceeds 34–35%.

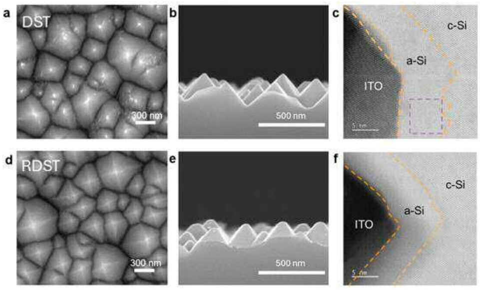

Figure 3: Pyramid morphology modification

The combination of the expertise at IET2 and IMD3 enables a combined experimental–theoretical strategy to accelerate the fundamental understanding of the underlying physical mechanisms and to guide process optimization.

Key tasks in this project:

1. **Set up a phase field model for heterogeneous crystallization of perovskite on textured surfaces:** Based on the existing implementation, include controllable surface energies at the substrate that are valid for arbitrary geometries, as well as a large number of relevant materials. Perform large-scale simulations for a wide spectrum of parameters to investigate the interplay of texture and process parameters on the crystallization of perovskite.
2. **Experimental validation of the simulation results based on the model:** Produce test samples to investigate the impact of texture, surface (TCO/SAM), and quenching on crystallization and compare the results with simulation results for validation.
3. **Define a roadmap for conformal wet-coating of perovskite on random pyramid texture:** Based on insight from (1) and (2), define a strategy for how to obtain a conformal coating using wet chemistry. Potential solutions could be a two-step wet process and/or adaptation of the quenching process.
4. **Develop a working approach for conformal wet-coating of perovskite on a random pyramid texture:** After the roadmap is defined, it should be systematically tested experimentally and supported by simulations. Optimize the process by improved experiments guided by detailed simulations.
5. **Develop a perovskite silicon tandem solar cell using the conformal wet-chemical process:** A high-efficiency perovskite silicon tandem solar cell will be demonstrated using the developed process. Optimization to achieve efficiency beyond 34% should be targeted.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Technologies - Helmholtz-Institute **Erlangen-Nürnberg** for Renewable Energy (IET-2 / HI ERN), Director: Prof. Dr. Karl Mayrhofer https://www.hi-ern.de/en
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Energy Materials and Devices - Photovoltaics (IMD-3), Director: Prof. Dr. Christoph Brabec https://www.fz-juelich.de/en/imd/imd-3
Specific **requirements**	M. Sc. in Physics, Chemistry, Materials Science, or a related discipline
For **project specific** questions please **contact**	Prof. Dr. Jens Harting, IET-2, j.harting@fz-juelich.de Dr. Kaining Ding, IMD-3, k.ding@fz-juelich.de

Research Project #13

AI-Enhanced Hierarchical Modeling of Water Electrolysis Cells (IET-3, IET-1 & IET-4)

Electrochemical devices such as electrolyzers, fuel cells, and batteries are central to the transition to renewable energy. Accurate modeling and simulation of these systems requires a comprehensive understanding of the complex physical processes involved and their interactions. Within these devices, multiple phenomena occur simultaneously across different length and time scales and within distinct functional layers, including multi-step electrochemical/chemical reactions, multi-phase transport in porous media, heat and mass transfer, and electrical potential distributions.

Recent advances in macro-homogeneous modeling have enabled coupled simulations of these processes, capturing multi-phase flow, electrochemical/chemical kinetics, and transport phenomena. However, many of these models rely on coarse approximations, empirical sub-models, or simplified representations of key phenomena due to the high computational cost of fully resolved simulations, from atomistic modeling through molecular dynamics to upper-scale modeling. As a result, these simulations often fail to capture the true coupled behavior of the mechanisms in the system, limiting both predictive accuracy and mechanistic understanding.

The primary objective of this PhD project is to integrate artificial intelligence (AI) models directly into macro-homogeneous simulations of electrolysis cells. Instead of resolving computationally expensive sub-scale phenomena within each iteration of the solution process, AI models will capture these behaviors with high fidelity, significantly reducing computational cost while retaining detailed accuracy. Applications include modeling complex multi-step reaction kinetics on electrode surfaces and/or multi-phase transport through porous structures. The AI models will be trained on sub-scale numerical simulations, atomistic/molecular dynamics modeling results, geometry-resolved simulations, and experimental datasets—including computed tomography (CT) or focused ion beam scanning electron microscopy (FIB-SEM) of electrode structures and cell performance measurements. These AI-enhanced models will be embedded within the macro-homogeneous Computational Fluid Dynamics (CFD) framework o*penFuelCell2*, enabling improved prediction of local properties and phenomena under various operating conditions. This approach will support the optimization of cell geometry, functional layer thicknesses, and material properties to maximize electrochemical performance and efficiency.

While the applicability of AI models has been demonstrated for individual physical phenomena[2], the transfer to multiphysical simulations, including those relevant for electrolysis cells, is still pending. The potential gain in computational speed provided by these models would unlock entirely new simulation capabilities and provide deeper insights into the underlying system behavior.

The dissertation research will be conducted in close collaboration with the Institute for Electrochemical Process Engineering (IET-4), and the Institute for Fundamental Electrochemistry (IET-1), providing access to high-quality experimental data and advanced characterization techniques. The AI–simulation interface will be fully integrated into the ongoing development of the open-source simulation framework o*penFuelCell2*, ensuring that the resulting methods are transferable and widely applicable to the broader electrochemical devices community. The specific tasks include:

Physics-based modeling and AI integration

- Develop AI surrogate models on sub-scale resolved simulations, atomistic models, molecular dynamics, and experimental data to improve the fidelity of coarse-grid models.
- Utilize experimental and simulation datasets, including CT/FIB-SEM-resolved electrode microstructures and cell performance measurements, to calibrate and validate the AI–physics models.
- Adapt hierarchical macro-homogeneous models for water electrolyzers, capturing coupled transport, electrochemical kinetics, and/or multi-phase flow processes.

- Implement AI–physics coupling interface with the o*penFuelCell2* framework to predict local electrochemical conditions and optimize cell performance.
- Conduct sensitivity analyses and surrogate modeling to identify key parameters that govern the overall performance of the electrolisys cell

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Technologies - Theory and Computation of Energy Materials (IET-3), Director: Prof. Dr. Michael Eikerling https://www.fz-juelich.de/en/iet/iet-3
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Energy Technologies - Fundamental Electrochemistry (IET-1), Director: Prof. Dr. Rüdiger- A. Eichel https://www.fz-juelich.de/en/iet/iet-1 Forschungszentrum Jülich, Institute of Energy Technologies - Electrochemical Process Engineering (IET-4), Director: Prof. Dr. Ralf Peters https://www.fz-juelich.de/en/iet/iet-4
Specific **requirements**	M.Sc. in (Electro-)Chemistry, Physics, Materials Science, Computational Science or in related disciplines. Experience in numerical simulations is essential. Prior experience with OpenFOAM would be an advantage. Proficiency in C++ and in Python or comparable programming languages is expected.
For **project specific** questions please **contact**	Dr. Thomas Kadyk (Head of the Physical Modeling and Diagnostics division), IET-3, t.kadyk@fz-juelich.de

[1] S. Zhang, S. Hess, H. Marschall, U. Reimer, S. Beale, W. Lehnert, openFuelCell2: A new computational tool for fuel cells electrolyzers, and other electrochemical devices and processes, Comput. Phys. Commun. 298 (2024) 109092.

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Research Project #14

Simulating Catalytic Interfaces for Chemical Hydrogen Storage (IET-3 & INW-1)

Background. Hydrogen plays a pivotal role as an energy carrier in the transition towards sustainable energy and industry systems [1]. Storage of hydrogen in either gas or liquid form is challenging and associated with high costs due to special requirements in container materials and storage conditions [2]. Liquid organic hydrogen carriers (LOHCs) are an attractive alternative to store hydrogen via chemical bonding in organic molecular structures, providing safe and economically feasible options for infrastructure compatibility [2,3]. During charging (hydrogenation), or discharging (dehydrogenation), hydrogen is incorporated into, or released from, the LOHC molecules via changes in process temperature and pressure at the surface of a catalyst material that is needed to achieve feasible hydrogenation/dehydrogenation rates. **New results show that the hydrogen turnover can be enhanced by applying an electrochemical potential at the catalyst surface**. It is assumed that the electrochemical environment modifies the interaction between catalyst and LOHC molecules and induces structural dynamics at the solid–liquid interface that facilitate the release of hydrogen. While the electrochemical LOHC activation has been demonstrated in experiments [4,5,6], fundamental understanding of the physicochemical interactions between LOHC molecules and electrified catalyst surfaces is still limited and systematic studies including theory and computation are required.

Goals. This Ph.D. project will model and simulate the interfacial interactions and phenomena between electrified platinum catalyst surfaces and liquid organic hydrogen carrier (LOHC) molecules, such as benzyltoluene. Using density functional theory (DFT) simulations, the hydrogenation and dehydrogenation mechanisms of LOHC molecules at the catalytic interface will be elucidated and the influence of the electrochemical environment on activation and degradation of LOHC molecules assessed. The theoretical investigations of this project at the *Institute of Energy Technologies: Theory and Computation of Energy Materials (IET-3)* will be closely aligned with experimental studies conducted simultaneously at the *Institute for a Sustainable Hydrogen Economy: Catalytic Interfaces for Chemical Hydrogen Storage (INW-1)*. Through combined theoretical and experimental assessment, fundamental understanding of the electric modulation effect in catalytic LOHC (de)hydrogenation will be achieved. The results of this project are expected to be of immediate relevance in chemical hydrogen storage by defining conditions for optimal process efficiency, selectivity, and durability.

Computational methods. Applying an electrochemical potential can tune the catalytic turnover during (de)hydrogenation of LOHC molecules in thermal catalytic processes [7]. We aim to reveal the fundamental principles underlying this effect using quantum-chemical DFT simulations for studying reaction pathways, intermediate molecular structures, and associated reaction barriers for the hydrogenation and dehydrogenation of LOHC molecules at electrified solid–liquid interfaces. The electrochemical environment will be simulated with the use of hybrid explicit/implicit solvation models in combination with advanced grand-canonical DFT schemes [8]. Concepts from chemical reactivity theory, such as frontier orbital analysis, will be used to identify descriptors for interfacial reactivity of LOHCs under electrochemical control and estimate the stability windows of LOHC molecules [9,10]. This workflow will not only provide essential insights for the design of optimized catalytic processes for hydrogen storage but also enable accelerated search for new LOHC candidates.

Tentative Work Plan. The Ph.D. student to be hired will first construct atomistic models of catalytic interfaces between a platinum catalyst surface and a liquid phase comprising LOHC molecules. The DFT framework will be used to predict the thermodynamic properties of the LOHC system. After validation of the simulation framework, the interfacial structures and transition states during LOHC (de)hydrogenation will be explored to gain insights into critical reaction steps and kinetic barriers. As an important advancement, the influence of the electrochemical reaction environment will be included by grand-canonical DFT and solvation methods and the impact of interface polarization on the catalytic reaction barriers will be analyzed. Finally, the stability properties of LOHC molecules at the charged catalyst surface will be determined, examining various possible decomposition pathways. The results from DFT simulations will be used to construct kinetic rate models for the catalytic LOHC (de)hydrogenation on Pt as a function of external control variables. The Ph.D. student will engage in a close collaboration with experimentalists at INW-1 to validate and leverage results from simulation and modelling in real-world experiments and applications. To conduct the theoretical studies, the Ph.D. student will access and utilize the cutting-edge supercomputers installed on the campus of Forschungszentrum Jülich.

Outcomes. This Ph.D. project will deliver a simulation and modelling workflow to describe the processes of (de)hydrogenation of LOHC molecules at electrified catalytic interfaces. The project results will be disseminated through presentation at international conferences and publication in recognized scientific journals. The resultant understanding will set the theoretical foundation of utilizing electrochemical control for tuning molecular interactions at catalytic interfaces for hydrogen storage technologies. Forschungszentrum Jülich provides an ideal environment for this project with a strong integration of theoretical and experimental research for driving the energy transition.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Technologies - Theory and Computation of Energy Materials (IET-3), Director: Prof. Dr. Michael Eikerling https://www.fz-juelich.de/en/iet/iet-3
Partners of the HITEC Project	Forschungszentrum Jülich, Institute for a Sustainable Hydrogen Economy - Catalytic Interfaces for Chemical Hydrogen Storage (INW-1), Director: Prof. Dr. Hans-Georg Steinrück https://www.fz-juelich.de/de/inw/unsere-bereiche/inw-1
Specific **requirements**	M.Sc. in computational chemistry or physics. Knowledge in physical chemistry and prior experience with first principles-based simulation approaches.
For **project specific** questions please **contact**	Dr. Tobias Binninger, IET-3, t.binninger@fz-juelich.de Dr. JiMun Yoo, INW-1, j.yoo@fz-juelich.de

[1] D. Guan *et al.* (2023) *Energy Environ. Sci.* 16, 4926-4943.
[2] P. M. Modisha *et al.* (2019) *Energy Fuels* 33, 2778-2796.
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[7] C. G. Vayenas *et al.* (1988) *J. Phys. Chem.* 92, 5083-5085.
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Research Project #15

Combining large scale atomistic simulations with neutron scattering experiments for understanding of interfacial dynamics of water, ligand and iron oxides for energy applications (IET-3 & JCNS-3)

At IET-3 we pursue research in theory and computation that complements experimental materials research on novel electrocatalysts. Crucial scientific challenges in this context are addressed with numerical atomistic modelling, either *ab initio* or molecular mechanics-based. These challenges encompass processes that alter structural, mechanical and thermodynamic properties of solid materials and their interfaces with the aqueous phase, including microscopic charge transfer, degradation via catalyst dissolution or support corrosion, and interfacial diffusion. To assure reliability of the computational workflows we develop accurate and efficient computational methodologies and evaluate their feasibility by comparison with experimental data provided by our partners. Among them, JCNS-3 applies neutron scattering and X-ray methods as a unique probe to characterize the structureand dynamics of materials over many length and time scales, studies energy systems in-situ and operando, as well as develops and operates neutron instruments at neutron sources.

Despite being omnipresent in various applications spanning fuel cells, heterogeneous catalysis and biomedicine, the dynamics of water molecules diffusing on nanostructured iron oxide surfaces are not yet well understood. This is in part because of the presence of organic ligand molecules that stabilize the nanostructured surfaces, producing complex interfacial behavior. Because a neutron favorably interacts with hydrogen, quasielastic neutron scattering (QENS), mastered at JCNS-3, is an ideal technique to investigate interfacial diffusion dynamics of hydrogen-containing species. It allows us to gain insight into the relaxation times, activation energies and geometry of motion of water molecules on nanoparticle surfaces. This information can be interpreted with the aid of atomistic simulations mastered at IET-3 and enabled by superior supercomputing facilities of the research center, particularly the exascale JUPITER supercomputer. This allows us to disentangle the diffusion dynamics of ligand molecules from that of light and heavy water molecules.

The aim of this project is to perform advanced, large-scale molecular dynamics simulations based on machine learning (ML) to interpret the neutron spectroscopy experiments on iron oxide nanoparticle powders. These nanoparticles will be synthesized according to a strategy well-established at JCNS-3, and stabilized with either citrate, lactic acid or diethylene glycol molecules, with samples equilibrated at different relative humidities of D_2O, which reflects a different number of water layers on the nanoparticle surface. The foreseen computational results will be integrated into the data analysis of the neutron spectroscopy data, in order to achieve a global understanding of the interfacial dynamics of D_2O and H_2O molecules. Part of the neutron data is already available from a running project; further neutron experiments shall be complemented by this project. Combining data from computation and experiment will allow to achieve new insights into interfacial dynamics of water-ligand-iron oxide surfaces.

This highly interdisciplinary and collaborative project will be executed by combining the long-standing experience of your hosts (IET-3 and JCNS-3) and collaboration partners. You will learn state-of-the-art high-performance simulation and data analysis techniques. Studies will be performed on world-class facilities at Forschungszentrum Jülich with the JUPITER exascale machine and world-wide available neutron scattering facilities as main resources.

Specific tasks are:

- to employ high-performance exascale supercomputing resources for nanoscale simulations of iron-oxide interfaces,
- to develop AI/ML force fields for use in computer-based simulations of iron-oxide comprising tens of thousands to millions of atoms and validate it against *ab initio* simulations on smaller scale models (up to a few hundreds of atoms),
- to perform neutron spectroscopy experiments at neutron sources worldwide including sample preparation and complementary physicochemical characterization (JCNS-3),
- to apply the devised force fields to large-scale molecular dynamics simulations of the particle-level processes such as interfacial diffusion, to provide support in interpreting the neutron scattering data,

- based on simulated and measured data to characterize diffusion mechanisms and identify differences of H_2O and D_2O diffusive properties at iron-oxide interfaces,
- to effectively collaborate on the topic with the internal and external partners,
- to publish results in peer-reviewed scientific journals and presentations at conferences and workshops.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Technologies - Theory and Computation of Energy Materials (IET-3), Director: Prof. Dr. Michael Eikerling, Computational Materials Modelling Division (Head: Dr. Piotr Kowalski) https://www.fz-juelich.de/en/iet/iet-3
Partners of the HITEC Project	Forschungszentrum Jülich, Jülich Center for Neutron Science - Neutron Analytics for Energy Research (JCNS-3), Director: Prof. Dr. Mirijam Zobel https://www.fz-juelich.de/en/jcns/jcns-3
Specific **requirements**	M.Sc. in Chemistry, Physics, Computational Materials Science, Geoscience or related disciplines; Experience in high performance computing as well as in X-ray or neutron scattering and data analysis will be an advantage; Good command of written and spoken English
For **project specific** questions please **contact**	Dr. Piotr Kowalski, IET-3, p.kowalski@fz-juelich.de (simulations/modelling) Prof. Dr. Mirijam Zobel, m.zobel@fz-juelich.de (neutron scattering, experiments)

Research Project #16

Digital-twin-guided design of CO_2 and bicarbonate electrolyzers through combined computational–experimental workflows (IET-4 & IET-3)

Electrochemical CO_2 conversion in membrane–electrode-assembly (MEA) electrolyzers is a promising approach for sustainable fuel and chemical production. However, current systems still face significant limitations—including carbon losses, mass-transport issues, and narrow operating ranges—that are even more challenging in emerging bicarbonate electrolyzers, which convert CO_2 directly from capture solutions. Increasing evidence indicates that local pH, ion transport, and membrane–electrode coupling are crucial factors affecting carbon efficiency and product selectivity, highlighting the need for a deeper mechanistic understanding. Integrating these systems with a validated digital-twin framework offers a new and powerful solution: by combining imaging, diagnostics, and multiscale modeling, digital twins can deliver continuous feedback, predictive insights, and real-time optimization. This integration has the potential to significantly improve the robustness, efficiency, and industrial viability of next-generation low-temperature CO_2 electrolyzers. [1]

This PhD project aims to develop a validated digital twin for CO_2 and bicarbonate electrolyzers, capable of accurately reproducing local electrochemical conditions—such as potential, pH, and reactant distribution—to optimize system performance. The model will support the development of design rules for advanced MEA components, including membrane selection, gas diffusion electrode architecture, and electrolyte formulations that improve selectivity and CO_2 utilization. Ultimately, this digital framework will provide feedback as well as prognostic and diagnostic insights to guide and interpret experimental behavior. [2,3]

The project will combine experimental and computational approaches from IET-4 and IET-3 into a unified workflow linking electrochemical testing, diagnostics, and multi-scale modeling. This integration will accelerate the design of next-generation electrolyzers and will also provide a transferable modeling framework for other reactive-capture electrochemical systems.

Through model–experiment feedback and optimization, the digital twin will undergo sensitivity analyses and surrogate modeling to identify key performance parameters such as diffusion layer thickness, membrane hydration, and catholyte composition. The optimized model will then guide the design of MEAs and operational strategies that maximize both CO_2 utilization efficiency and product selectivity (targeting over 80%), while also minimizing cell voltage. This approach will lead to improved performance and a deeper mechanistic understanding of CO_2 electrolysis. The specific tasks, organized into physics-based modeling and experimental validation parts, are:

Physics-based modeling (IET-3)

- Develop hierarchical 1D–3D electrochemical multiphysics models for CO_2 and bicarbonate cells, accounting for charge transport, species migration, and water management.

- Incorporate mechanistic sub-models for $CO_2/HCO_3^-/CO_3^{2-}$ equilibria, local CO_2 regeneration, and competing hydrogen evolution.

- Embed all components into a reusable digital-twin framework calibrated using experimental data (EIS, polarization curves, tomography) that provides feedback to the experimental setup.

Experimental validation (IET-4)

- Fabricate and test MEAs for conventional CO_2 and bicarbonate electrolysis, systematically varying membranes (PEM, BPM), electrode structures, and electrolytes suggested by the models.

- Perform in-depth electrochemical characterization (I–V curves, faradaic efficiencies, CO_2 utilization, and impedance analysis) and 3D structure imaging for model validation.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Technologies - Electrochemical Process Engineering (IET-4), Director: Prof. Dr. Ralf Peters https://www.fz-juelich.de/en/iet/iet-4
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Energy Technologies - Theory and Computation of Energy Materials (IET-3), Director: Prof. Dr. Michael Eikerling https://www.fz-juelich.de/en/iet/iet-3
Specific **requirements**	M.Sc. in (Electro-)Chemistry, Physics, Materials Science, Computational Materials Science or in related disciplines. Experience in numerical simulations would be an advantage.
For **project specific** questions please **contact**	Dr. Joachim Pasel (Head of the Synthetic Fuels Department), IET-4, j.pasel@fz-juelich.de Dr. Thomas Kadyk (Head of the Physical Modeling and Diagnostics division), IET-3, t.kadyk@fz-juelich.de

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2. Khiarak, B. N. *et al.* Integrated Carbon Dioxide Capture and Electrochemical Conversion: Chemistry, Electrode and Electrolyzer Design, and Economic Viability. *Advanced Energy Materials* **n/a**, e02564.

3. McLaughlin, D., Bierling, M., Mayerhöfer, B., Schmid, G. & Thiele, S. Digital Twin of a Hierarchical CO2 Electrolyzer Gas Diffusion Electrode. *Advanced Functional Materials* **33**, 2212462 (2023).

Research Project #17

Experimental and Simulative Development of an Efficient Direct Air Capturing (DAC) Process (IET-4 & IMD-2)

Direct Air Capture (DAC) comprises technologies designed to separate CO_2 from ambient air, thereby generating negative emissions. These negative emissions can offset CO_2 from hard to abate sectors and can therefore play a vital role in meeting the climate targets of the Paris Agreement. [1]. The latest IPCC report further highlights the importance of employing DAC to achieve these targets [2]. Consequently, there is currently considerable public interest in this technology, although several research challenges remain in order to further advance its development.

The DAC technology with the highest Technology Readiness Level is the adsorption-based approach. A key area for improvement lies in the adsorbents used in DAC systems. Adsorption capacity, selectivity toward CO_2, and long-term stability are of central importance for overall process performance. To date, energy demand and costs represent the main hindrance to a global roll-out of DAC. Since the range of commercially available adsorbents remains limited to a single material, the production of novel adsorbents at a scale that allows thorough testing is essential. Moreover, bench-scale testing can provide new insights into the heat and mass transfer characteristics of these adsorbents, which cannot be investigated adequately at lab-scale.

Such a bench-scale “mini-plant” is currently under construction at the Institute of Energy Technologies (IET-4), which is specially designed based on preliminary process analysis [3] and to be commissioned in 2026. Standard as well as novel solid sorbents will be tested, which are being developed and produced in small to medium-sized batches at the Institute of Energy Materials and Devices (IMD-2). This interdisciplinary approach is required to identify most promising operation and respective materials since optimization is only possible in a holistic view.

Within the framework of this interdisciplinary PhD project, a further milestone in DAC research is to be achieved, building upon the recent studies already completed. The research will cover multiple levels, including material synthesis, experimental characterization in lab- and bench-scale, and process simulation.

Tasks to be completed during this PhD project include:

- Production of sorbents on a kilogram scale with reproducible quality and in a form suitable for use in the DAC miniplant.
- Operation of the DAC pilot plant using the self-produced sorbents as well as reference materials and characterization of their performance under operating conditions.
- Thermodynamic modeling of the DAC process with varying material properties and operation conditions.
- Development of an energy-optimized operational strategy and respective material requirements for large-scale DAC plants based on the insights gained.

The overarching goal of this project is to advance the understanding of the sorbents utilized and to enhance the overall DAC process, thereby increasing the technical efficiency and economic viability of DAC technology.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Technologies - Electrochemical Process Engineering (IET-4), Director: Prof. Dr. Ralf Peters https://www.fz-juelich.de/en/iet/iet-4
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Energy Materials and Devices – Materials synthesis and Processing (IMD-2), Director: Prof. Dr. Wilhem Albert Meulenberg https://www.fz-juelich.de/en/imd/imd-2
Specific **requirements**	Background in chemical engineering, material engineering, mechanical engineering, environmental engineering or comparable First Lab experience First modelling experience preferable
For **project specific** questions please **contact**	Dr. Nils Beltermann, IET-4, n.beltermann@fz-juelich.de Dr. Stefan Baumann, IMD-2, s.baumann@fz-juelich.de

[1] United Nations Framework Convention on Climate Change, Paris Agreement, United Nations, 2015

[2] IPCC, Synthesis Report of the IPCC Sixth Assessment Report (AR6): Climate Change 2023

[3] A. S. Jajjawi et al., Exploring Weather Impacts on Direct Air Capture Through Process and Techno-Economic Modeling, 2025

Research Project #18

Physicochemical investigations of the electric double layer of protic ionic liquids as novel electrolytes for high-temperature polymer fuel and electrolysis cells (IET-4 & INW-1)

Polymer fuel cells and electrolysis cells are pivotal technologies for clean power generation and green hydrogen production. Yet their performance and durability continue to be constrained by the low to moderate operating temperatures required by conventional polymer electrolytes and aqueous environments. Typical operation below 80 °C limits reaction kinetics, increases susceptibility to catalyst poisoning, imposes strict humidification control, and reduces overall system robustness. Overcoming these temperature constraints is therefore essential for enabling more efficient and reliable electrochemical devices.

At IET-4 and INW-1, we investigate the fundamental physicochemical properties of protic ionic liquids (PILs) as promising electrolytes for future intermediate and high-temperature fuel and electrolysis cells (100-180 °C). Their intrinsic thermal stability, negligible vapor pressure, and non-flammability allow PILs to function well beyond the temperature limits of water-based electrolytes. When incorporated into polymer fuel cells or electrolysis cells as proton-conducting electrolytes embedded in a polymer matrix, PILs can enable high-temperature operation, which would increase the overall system efficiency and thus reduce the costs of fuel and electrolysis cells [1,2].

A key factor in realizing these advantages lies in understanding and rationally engineering the electric double layer (EDL) that forms between ILs and Pt electrodes. PILs create highly ordered, ion-rich interfacial layers that differ radically from those formed in traditional proton-exchange environments [3]. These structured EDLs govern charge distribution, adsorption processes, and the activation barriers of reactions central to fuel-cell and electrolysis performance. At elevated temperatures, changes in PIL mobility, water content, and interfacial structuring can significantly influence the rates of hydrogen oxidation, oxygen reduction, and water-splitting reactions on Pt.

Despite the promise of ILs for high-temperature operation, fundamental questions remain unresolved. What is the EDL structure on the nanoscale? How is it influenced by changes in water content and electric potential? Is there a preferential tendency for blocking catalytically active sides of specific anion-cation combinations? And, importantly, how does the structure of the EDL influence the relevant electrochemical processes at the catalyst interface?

This project aims to elucidate the EDL formed between (P)ILs and Pt electrodes in model cells combining electrochemical methods with *in situ* Raman spectroscopy and X-ray diffractometry/reflectometry (XRD/XRR) [4,5]. The study focusses on a systematic selection of ILs that vary in cation type, anion chemistry, hydrophobicity, acidity and thus in proton availability. Pt electrodes—polycrystalline disks, (ordered) thin films, or single crystals—are prepared with high surface cleanliness to minimize structural ambiguities. These electrodes are incorporated into customized electrochemical cells equipped with optical and X-ray transparent windows as well as precise temperature and atmosphere control to allow operation from room temperature to the target operation temperatures above 100 °C.

Baseline electrochemical characterization using cyclic voltammetry and impedance spectroscopy provides an initial fingerprint of IL–Pt interactions by identifying ion adsorption features, potential stability windows, and temperature-dependent changes in interfacial capacitance. These data guide the subsequent spectroscopic measurements. *In situ* Raman spectroscopy is then used to probe molecular-level interactions in the EDL, beginning with bulk IL characterization to establish reference vibrational signatures associated with ion pairing, hydrogen bonding, and structural order. Potential-controlled *in situ* Raman measurements at the Pt surface reveal how IL ions reorganize in response to electrode polarization, including changes in adsorption, coordination, and formation of an ordered structure based on anion-cation layering. Surface enhanced Raman spectroscopy (SERS) based on the use of plasmon active nanoparticles will be employed to differentiate vibrational signatures of the interface from the bulk.

Complementing Raman spectroscopy, *in situ* XRR is employed to resolve the spatial structure and ordering of ILs near the Pt surface. Initial bulk XRD measurements identify intermolecular interactions and the structure of solvation shells. Surface-sensitive XRR measurements then map interfacial layering, ion stratification, and molecular orientation within the first few nanometres above the Pt electrode (i.e., within the EDL). By applying potentials during experiments, the experiments monitor how electrochemical polarization compresses or reorganizes near-surface ordering.

The final phase integrates the complementary experimental measurements with theoretical models obtained by molecular dynamics (MD) and density functional theory (DFT) to reveal correlations between PIL chemistry, EDL structure, and electrochemical performance. Based on these findings, a model will be established predicting the most promising PIL composition to be used in test cells after embedding in a thermally stable polymer.

The project will be conducted at the state-of-the-art experimental research facilities of Forschungszentrum Jülich and large scale research facilities such as synchrotrons ERSF and PETRA III. The dissertation research will be conducted in close collaboration with internal project partners of various institute on the campus and the RWTH Aachen University as well as with leading research groups in electrocatalysis and physical chemistry in Europe, South Korea and South Africa.

The specific tasks of the project are:

- to employ cutting-edge nanoscale experimental methods for the investigation of the EDL of PILs
- to develop dedicated *in situ* model cells for Raman spectroscopy and XRR
- to evaluate the applicability of *ab initio* models for the description of electrochemical reactions
- to predict optimized electrolyte compositions for efficient high-temperature PEM fuel and electrolysis cells
- to effectively collaborate with the internal and external partners.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Technologies - Electrochemical Process Engineering (IET-4), Physicochemical lab (PCL), Director: Prof. Dr. Ralf Peters https://www.fz-juelich.de/en/iet/iet-4
Partners of the HITEC Project	Forschungszentrum Jülich, Institute for a Sustainable Hydrogen Economy - Catalytic Interfaces for Chemical Hydrogen Storage (INW-1), Director: Prof. Dr. Hans-Georg Steinrück https://www.fz-juelich.de/de/inw/unsere-bereiche/inw-1
Specific **requirements**	M.Sc. in Physics, Chemistry or in related disciplines
For **project specific** questions please **contact**	Dr. Christian Rodenbücher, IET-4, c.rodenbuecher@fz-juelich.de

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4. Steinrück, H.-G.; Cao, C.; Tsao, Y.; Takacs, C.J.; Konovalov, O.; Vatamanu, J.; Borodin, O.; Toney, M.F. The nanoscale structure of the electrolyte–metal oxide interface. *Energy Environ. Sci.* **2018**, *11*, 594–602, doi:10.1039/C7EE02724A.
5. Horowitz, Y.; Steinrück, H.-G.; Han, H.-L.; Cao, C.; Abate, I.I.; Tsao, Y.; Toney, M.F.; Somorjai, G.A. Fluoroethylene Carbonate Induces Ordered Electrolyte Interface on Silicon and Sapphire Surfaces as Revealed by Sum Frequency Generation Vibrational Spectroscopy and X-ray Reflectivity. *Nano Lett.* **2018**, *18*, 2105–2111, doi:10.1021/acs.nanolett.8b00298.

Research Project #19

Examination and Correlation of Radiation Damage Effects in Materials Arising from Fission and Fusion Energy Applications (IFN-2 & IFN-1)

The accelerated shift towards carbon neutrality coupled with concerns over energy sovereignty have refocused attention upon nuclear energy technology, particularly conventional fission and future fusion-based forms. Invariably, both energy systems demand materials that can withstand extreme conditions of high temperatures and intense radiation damage for both safe *in operando* performance and as final disposed waste materials. Refractory materials such as those based on uranium, tungsten and zirconium have high melting points with strong radiation tolerances, which makes them suitable for fission and fusion energy applications. Nevertheless, they are still susceptible to material degradation and loss of structural integrity due to variable response from dynamic temperature and radiation doses. These materials are crucial to both fission and fusion energy applications in relation to spent nuclear fuel stability or first wall material candidates in fusion. Understanding and correlating radiation damage effects from both low to high temperatures, and radiation doses, is critical for their safe usage and final disposal. This consequently enables enhanced understanding of critical materials used in both fission and fusion applications, guiding their safe use, deployment and final disposal.

The PhD project is a joint experimental venture between the Institute of Nuclear Waste Management (IFN-2) and Institute of Plasma Physics – Nuclear Fusion (IFN-1) at Forschungszentrum Juelich GmbH. The project will harness the manufacturing and unique radioactive handling facilities of INF-1 and IFN-2 to fabricate high refractory oxide and alloy materials, perform irradiation damage and post-characterization in order to develop enhanced understanding of such materials for fission and fusion applications and disposal. High resolution measurements will involve the use of neutron and synchrotron X-ray scattering techniques, such as diffraction and spectroscopy based, to assess structural changes to materials. Further deployment of scanning and transmission electron microscopy techniques will also be used to assess microstructural changes across variable temperature dose scales. The PhD candidate will explore uranium, tungsten and zirconium oxide and alloy-based material compositions and further seek to explore their behaviour as low and high entropy materials. The overall goal will be to develop a structure-physics based description of radiation damage in fusion and fission-based materials that can be linked across low- to high-dose radiation damage regimes. With support of the supervisors from the participating institutes, the PhD candidate will subsequently develop world leading expertise jointly in nuclear material handling, fabrication, characterization, atomistic simulations and computation analysis.

The Institute of Nuclear Waste Management (IFN-2) focuses on researching materials and processes relevant to the safe management of radioactive waste and its eventual final disposal. The research at IFN-2 is multidisciplinary, although typically the core focus is nuclear related, the institute combines radio-, geo- and materials chemistry disciplines in addition to computation and simulation synergistically. Research at IFN-2 covers the complete post-operative nuclear reactor cycle, from the initial waste generation, such as the discharge of SNF from the reactor core to its eventual disposal in a geological repository, including research examining the long-term safety behaviour. IFN-2 research further supports unresolved issues prior to waste disposal but also supporting general nuclear safety for instance pre-disposal planning, and research on international safeguards for instance supporting the International Atomic Energy Agency (IAEA) among other organisations. Inevitably, many material types encountered in nuclear waste management bear pertinence beyond this field, such as complex oxides, high entropy alloys and materials for hydrogen evolution. As such, the institute pursues research that is not just nuclear relevant but also societally.

The Institute of Plasma Physics – Nuclear Fusion (IFN-1) at Forschungszentrum Jülich has its research goals aligned with the national and European fusion programs. The roadmap of the institute is towards engineering and developmental activities for a fusion reactor in Germany, specifically focusing on Plasma Wall Interaction (PWI) studies for fusion reactors, material and component development, diagnostics development and qualification of first wall materials. The institute has dedicated groups working on PWI studies on linear plasma devices, experimental tokamaks, W-7X stellarator and modelling of the results. Additionally, to qualify materials under reactor relevant conditions, a high temperature materials laboratory with controlled areas for testing and qualification of irradiated materials including study of radiation damage, plasma exposures and high heat flux testing is being developed and modernized.

The specific tasks of the PhD Candidate are:

- To manufacture high purity refractory materials using solid state sintering techniques
- Performing accelerator based ion-irradiations
- Post fabrication and irradiated materials characterization, using state of the art, high resolution X-ray and neutron diffraction, X-ray absorption spectroscopy in addition to electron microscopy techniques.
- Perform radiation damage-based simulations and modelling.
- To effectively collaborate with internal and external partners.
- Dissemination of scientific results in the form of scientific conferences and written publications to medium to high impact journals.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Fusion Energy and Nuclear Waste Management – Nuclear Waste Management (INF-2), Director: Prof. Dr. Dirk Bosbach – Nuclear Waste Management Solid State Chemistry group, Head: Dr. Gabriel L. Murphy https://www.fz-juelich.de/en/ifn/ifn-2
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Fusion Energy and Nuclear Waste Management – Plasma Physics (IFN-1), Director: Prof. Dr. Christian Linsmeier, Plasma Wall Interactions – Materials, Head: Prof. Dr. Bernhard Unterberg https://www.fz-juelich.de/en/ifn/ifn-1
Specific **requirements**	M.Sc. in Chemistry, Physics, Materials Science or in related disciplines. Prior knowledge and experience in the nuclear field or radiation physics would be advantages but not essential
For **project specific** questions please **contact**	Dr. Gabriel L. Murphy, IFN-2, g.murphy@fz-juelich.de Dr. Rahul Rayaprolu, IFN-1, r.rayaprolu@fz-juelich.de

Research Project #20

Connecting Microstructural Evolution to the Effective Properties of Materials Using Lattice-Boltzmann Simulations and Machine Learning (IFN-2 & JSC)

Many engineering and energy applications, including fuel cells and batteries, heterogeneous catalysis, subsurface hydrogen extraction, and nuclear waste disposal systems, require a comprehensive understanding of porous microstructural evolution under coupled multiphase flow and chemical reactions [1,2,3]. The evolution of these microstructures critically influences the thermal, flow, and chemical properties of the system, thereby determining the overall system's performance and reliability.

However, establishing quantitative relationships between the evolving topological features of these complex microstructures and their corresponding effective properties remains a significant numerical challenge. Classical correlations, such as the Kozeny-Carman, Archie's, and Quirk-Millington equations, often fail to describe systems undergoing dynamic-topological, multiphase-flow, and chemical transformations, where assumptions of homogeneity, isotropy, and steady-state transport no longer hold. In these evolving microstructures, topological changes arising from processes such as precipitation or dissolution and interaction among different phases lead to nonlinear and time-dependent variations in transport pathways that cannot be captured by classical relationships.

High-fidelity numerical simulations, including using Lattice-Boltzmann methods, have advanced our ability to resolve these processes at the micro scale [2]. Nevertheless, there is currently no efficient Lattice-Boltzmann solver capable of handling coupled multiphase flow and chemical reactions, especially of treating the triple-point problem, i.e., locations, where solid, fluid, and gaseous media meet, in a numerically stable manner. Existing solvers often adopt simplified representation of chemical reactions, which may lead to inaccurate predictions of topological changes [4]. Moreover, while Lattice-Boltzmann simulations can provide valuable insights, relying solely on high-fidelity computations is prohibitive for exploring large parameter spaces.

To overcome these limitations, this project aims to develop an efficient reactive multiphase Lattice-Boltzmann solver at microscale, and a machine-learning based framework to extend correlation between various topologies and effective properties. We also plan to provide an open-source implementation of the framework for the broader scientific community. The approach will be validated using our recent microfluidic experimental data [3].

Tasks of the PhD project are:

- **WP-1**: Development of a parallel, reactive multiphase flow solver that combines a scalable multi-species Lattice-Boltzmann solver (e.g., from the m-AIA framework [preferred] [2,5], Palabos) and a thermodynamics-based chemical solver (e.g., Reaktoro [preferred] [6], PhreeqC).
- **WP-2**: Development of a machine-learning based framework to correlate microstructural topologies with their effective properties, incorporating generative AI approaches.

Once established, this framework will allow the design of porous microstructures to enhance fuel cell and battery performance, control chemical reactions in subsurface systems for optimized hydrogen production and ensure safety in nuclear waste disposal.

We offer:

- An interdisciplinary research team, consisting of computational science and engineering, geoscience, and geochemistry experts, embedded into an international environment
- Excellent scientific instrumentation, including exascale high-performance computing infrastructure and a cutting-edge radioactive-enabled microscopy laboratory
- Opportunities to attend national and international conferences, and to interact with international collaborators

- Payment and social benefits based on the labor agreement for the public sector employment (TVöD)

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Fusion Energy and Nuclear Waste Management - Nuclear Waste Management (INF-2), Director: Prof. Dr. Dirk Bosbach, Reactive Transport group, Head: Dr. Jenna Poonoosamy https://www.fz-juelich.de/en/ifn/ifn-2
Partners of the HITEC Project	Forschungszentrum Jülich, Jülich Supercomputing Centre (JSC), Directors: Prof. Dr. Dr. Thomas Lippert and Prof. Dr. Kristel Michielsen, Simulation and Data Lab "Fluids & Solids Engineering", Head: Dr. Andreas Lintermann https://www.fz-juelich.de/en/jsc
Specific **requirements**	MSc in computational science and engineering, computational geoscience, physics, mathematics, or related discipline with a focus on computational flow in porous media with chemical reactions
For **project specific** questions please **contact**	Dr. Ryan Santoso, IFN-2, r.santoso@fz-juelich.de Dr. Jenna Poonoosamy, IFN-2, j.poonoosamy@fz-juelich.de Dr. Andreas Lintermann, JSC, a.lintermann@fz-juelich.de

[1] Detmann, B. (2021). Modeling chemical reactions in porous media: a review. *Continuum Mechanics and Thermodynamics*, *33*(6), 2279-2300.

[2] Lintermann, A., & Schröder, W. (2020). Lattice–Boltzmann simulations for complex geometries on high-performance computers. *CEAS Aeronautical Journal*, *11*(3), 745-766.

[3] Poonoosamy, J., Santoso, R., Kaspor, A., Wegner, L., Dagnelie, R. V., & Miron, G. D. (2025). Microfluidic experiments to rationalize coupled mineral dissolution and precipitation with gas exsolution. *Geochimica et Cosmochimica Acta*.

[4] Alamian, R., Nayak, A. K., & Shadloo, M. S. (2025). CooLBM: A GPU-Accelerated Collaborative Open-Source Reactive Multi-Phase/Component Simulation Code via Lattice Boltzmann Method. *Computer Physics Communications*, 109711.

[5] Lintermann, A., Meinke, M., & Schröder, W. (2020). Zonal Flow Solver (ZFS): a highly efficient multi-physics simulation framework. *International Journal of Computational Fluid Dynamics*, *34*(7-8), 458-485.

[6] Leal, A. M. (2015). Reaktoro: An open-source unified framework for modeling chemically reactive systems. *URL: https://reaktoro.org*.

Research Project #21

Microstructure-driven rejuvenation of Li-ion cathodes enabled by in situ microscopy and controlled annealing (IMD-1 & ER-C-1)

Rechargeable lithium-ion batteries remain the backbone of electrified mobility and stationary storage, yet cathode sustainability is limited by structural degradation, elemental scarcity. Layered oxides such as Lithium Nickel Manganese Cobalt Oxide (NMC) and Lithium Nickel Cobalt Aluminum Oxide (NCA) progressively lose electrochemical performance through grain-boundary decohesion [1], oxygen release, cation disorder, and surface rock-salt formation [2]. These phenomena generate impedance and capacity loss long before chemical exhaustion occurs. Conventional recycling restores composition but not the nanoscale order enabling redox. The central scientific question therefore shifts from “how to recover materials” to “how to heal the specific microstructural and interfacial defects that control reversibility”.

As production volumes accelerate, direct cathode rejuvenation could yield the largest environmental and economic impact among circular technologies, but the mechanistic understanding required to guide it remains fragmentary. Recent reactivation approaches have demonstrated high process efficiency. For example, flash Joule heating (FJH) – a millisecond-scale high-current pulse treatment recently applied to spent cathodes – achieves rapid relithiation and impurity removal with a strong life-cycle advantage [3]. Yet, despite its promise, FJH exemplifies a process-first strategy: it emphasizes throughput and energy efficiency, while the underlying atomic-scale repair mechanisms remain largely undefined.

The proposed project therefore pursues a complementary, mechanism-first and microscopy-anchored route. Rather than optimizing an imposed process, it starts from the diagnosis of atomic failure motifs and derives targeted treatments that specifically heal them. To this end, the project will be conducted jointly by IMD-1 and ER-C-1. IMD-1 provides a versatile suite for *in situ* process studies, including a MEMS-based µReactor for controlled-atmosphere heating, an *in situ* TEM heating/biasing holder, µCT for three-dimensional crack tomography, SIMS, EBSD, TKD, glow-discharge and Knudsen spectroscopy, TGA/DTA/DSC, and *in situ* mechanical and electrochemical hydrogen-charging setups. ER-C-1 contributes world-leading aberration-corrected S/TEM (HAADF/ABF/iDPC), 4D-STEM phase and strain mapping, and spectroscopy (EELS/EDS) techniques for atomic-scale characterization of defects, irreversible phase transition and transition metal valence state change in spent and *in situ* regenerated cathodes. Together, these instruments enable controlled thermal or chemical rejuvenation and multiscale diagnosis across atomic, micro-, and mesoscale dimensions.

The methodological foundation of the project is a quantitatively controlled, atmosphere-programmed thermal relithiation and defect-healing strategy, using the µReactor and *in situ* TEM as discovery platforms. In the µReactor, individual particles or small ensembles are heated under defined O_2/Ar ratios and subsequently quickly cooled, mimicking flash-type thermodynamics while enabling direct observation. Thin Li_2CO_3 or $LiPO_4$ coatings provide lithium chemical potential for relithiation where needed. Complementary *in situ* TEM heating experiments on site-specific lamellae resolve the evolution of cation ordering, oxygen vacancy annihilation, and grain-boundary reconstruction in real time via STEM imaging, 4D-STEM mapping, and EELS fine structure. These datasets provide the mechanistic basis for process design and for quantifying the relation between thermal exposure, oxygen potential, Li availability and structural healing.

The project’s conceptual inspiration originates from W. Chen et al. [3], who demonstrated solvent-free FJH relithiation as a rapid, energy-lean reactivation route. While their work defines a new processing benchmark, the present study addresses the missing mechanistic layer: it identifies what microstructural transformations must occur and how they can be induced in a controlled manner. By exploiting the fine control of the µReactor and *in situ* TEM, we will parameterize the key variables – temperature, partial pressure of oxygen, dwell time, and lithium activity – and produce a transferable defect-function atlas. The mechanistic insights obtained at the microscale will later guide cooperative experiments using high-power or flash-like setups to verify scalability.

The doctoral research will proceed through five coordinated work packages integrating microscopy, process design, and correlative analytics:

WP1 – <u>Multiscale diagnosis:</u> Structural and chemical mapping of aged cathodes using aberration-corrected STEM/EELS/EDS to quantify rock-salt thickness, cation disorder, and oxygen-vacancy gradients. Complementary FIB-SEM and µCT tomography as well as TKD/EBSD will capture mesostructural cracking. The output is a defect taxonomy ranked by frequency and relevance.

WP2 – <u>Targeted repair via µReactor and *in situ* TEM:</u> design of atmosphere-programmed relithiation and interface-healing using controlled O_2/Ar flows and solid lithium precursors. Heating profiles will be optimized ordering recovery with minimal coarsening. *In situ* TEM will quantify ordering kinetics and interface retreat; TGA/DSC, SIMS, and glow-discharge spectroscopy will assess lithium mobility and reaction thermodynamics. Femtosecond laser hating in situ in the TEM in combination with the new dynamic TEM may allow observation of rejuvenation with µs to ns temporal resolution providing unique insights into the rejuvenation process.

WP3 – <u>Feedback validation:</u> post-treatment analyses combining high-resolution microscopy, EELS redox mapping, and electrochemical impedance spectroscopy (EIS), complemented by cyclic voltammetry (CV), and open-circuit voltage hysteresis as proxies for charge-transfer resistance and reversibility. The correlations between structure, repair, redox state, and impedance will define a predictive structure-property map.

WP4 – <u>Durability and micro-mechanical stability:</u> In situ TEM EIS and intermittent *in situ* mechanical tests during slow cycling and thermal loading will monitor the persistence of rejuvenated structures. Complementary XRD, Knudsen and gas-release spectroscopy will detect any secondary phases. The target is stable impedance and ordering over at least 300 low-rate cycles.

WP5 – <u>Transfer and proof-of-concept scaling:</u> translation of optimized conditions (T, pO_2, Li dose, dwell) to rapid thermal or resistive micro-boat treatments. Collaboration with partners possessing flash-heating or Joule-heating capabilities will demonstrate a proof-of-concept on a relevant gram-scale, verifying scalability of the mechanism-derived recipes. Thermal energy savings vs. fresh synthesis (calcination) will be evaluated via TGA/DSC.

By uniting the *in situ* and correlative infrastructures from IMD-1 and ER-C-1, this work will establish the first mechanistically validated playbook for microstructure-led rejuvenation of Li-ion cathodes. Its quantitative description of defect healing, verified by impedance and redox proxies, lays the foundation for subsequent flash-like or high-throughput demonstrations, offering a scalable path to circular energy-storage materials.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Materials and Devices – Structure and Function of Materials (IMD-1), Director: Prof. Dr. Ruth Schwaiger https://www.fz-juelich.de/en/imd/imd-1
Partners of the HITEC Project	Forschungszentrum Jülich, Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons – Physics of Nanoscale Systems (ER-C-1), Director: Prof. Dr. Rafal Dunin-Borkowski https://www.fz-juelich.de/en/er-c/er-c-1
Specific **requirements**	M.Sc. in materials science, physics, physical chemistry, or related with strong solid-state focus – Experience in electron microscopy and/or battery materials
For **project specific** questions please **contact**	Dr. Nicolas J. Peter, IMD-1, n.peter@fz-juelich.de Penghan Lu, ER-C-1, p.lu@fz-juelich.de

[1] S. Sharifi-Asl *et al*. “Revealing Grain-Boundary-Induced Degradation Mechanisms in Li-rich Cathode Materials” Nano Lett. 20(2), 1208-1217 (2020)

[2] C. Xu *et al.* “Bulk fatigue induced by surface reconstruction in layered Ni-rich cathodes for Li-ion batteries” Nat. Mater. 20, 84-92 (2021)

[3] W. Chen *et al.* “Nondestructive flash cathode recycling” Nat. Commun. 15, 6250 (2024)

Research Project #22

Performance & Systems Impact of Emerging Photovoltaic Technologies (IMD-3 & ICE-2)

Introduction & Novelty

The transition to a sustainable energy system depends on widespread adoption of renewable energy sources. Photovoltaics (PV) are expected to account for nearly 80% of all new renewable electricity capacity by 2030. Although silicon-based PV technology is well-established, emerging technologies such as perovskite, organic PV, and silicon-perovskite tandems offer the potential for greater efficiency and reduced manufacturing costs. However, the long-term performance and system integration implications of these novel PV technologies remain largely unexplored. This project addresses this gap by combining the detailed outdoor performance characterization of emerging PV modules with the system-level analysis of their potential impact on German and European energy systems. This analysis considers performance as well as the security of the material supply chain. The project's novel approach integrates granular, module-level data with macro-level energy system modeling, incorporating performance degradation and acclimatization effects that are crucial for reliable system assessment. This integration will provide a more realistic assessment of the viability and resilience of future renewable energy systems.

Project Description & Work Packages

This project will be undertaken by a PhD candidate jointly supervised by researchers at IMD-3 and ICE-2. The PhD candidate will spend time at both institutes, facilitating knowledge transfer and ensuring effective collaboration.

- **WP1: Outdoor Performance Monitoring (IMD-3)**: Establish and maintain a comprehensive monitoring campaign of standard (Si) and emerging (Si/Perovskite, Organic, etc.) PV modules at IMD-3's outdoor testing facility. This includes continuous monitoring of weather parameters (global/diffuse irradiance, temperature, wind) and electrical performance (IV curves, MPP tracking).

- **WP2: Data Analysis & Performance Modelling (IMD-3):** Develop robust data processing and analysis methods to account for outdoor data noise and variability. This will involve analyzing the influence of irradiance, spectral effects, and temperature on module performance. Crucially, the work will focus on identifying and modelling acclimatization effects, seasonal performance variations, and degradation mechanisms in both standard and emerging PV technologies.

- **WP3: Material Requirements and Supply Chain Analysis (ICE-2):** In parallel with performance data generation, the PhD candidate will work with ICE-2 to analyze the material requirements for each PV technology, per kWh generated, and assess the associated supply chain vulnerabilities and geopolitical dependencies. This will involve a literature review and implementation within the ETHOS model suite [5] to derive meaningful scenarios for supply options.

- **WP4: System-Level Impact Assessment (ICE-2):** Utilizing the performance and degradation models developed at IMD-3, and material data from WP3, ICE-2 will integrate these findings into its ETHOS model suite [5], which will involve different open-source tools like ETHOS.RESKit [4] and ETHOS.FINE [3]. This will enable assessment of the potential for new PV technologies to contribute to German/European energy security, considering both cost and resilience of supply chains. Focus will be on identifying scenarios where emerging PV technologies can enhance security of supply and reduce reliance on critical materials.

- **WP5: Dissemination and Reporting (Joint):** Active participation in conferences, workshops, and publications to disseminate research findings. Preparation of regular project reports and a final PhD thesis.

Research Context & References

The project builds upon existing research at IMD-3 on outdoor PV module characterization and degradation modelling [1,2] as well as its network within SolarTab. ICE-2’s expertise in energy systems modelling and the ETHOS model suite provides a strong foundation for the system-level analysis, which was and is contributing to several flagship reports of the IEA [6]. Recent publications highlight the urgent need for a comprehensive understanding of emerging PV technologies [8, …], and the importance of supply chain security for renewable energy deployment [9, …]. This project directly addresses these challenges by combining detailed module characterization with system-level analysis, providing a more holistic, technology-rich assessment of the potential of emerging PV technologies. The project directly supports the goals of the German energy transition ("Energiewende") and contributes to the development of a sustainable and resilient energy system.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Materials and Devices - Photovoltaics (IMD-3), Director: Prof. Dr. Christoph Brabec https://www.fz-juelich.de/en/imd/imd-3
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Climate and Energy Systems - Jülich Systems Analysis (ICE-2), Director: Prof. Dr.-Ing. Jochen Linßen https://www.fz-juelich.de/en/ice/ice-2
Specific **requirements**	Affinity for modelling and simulation works. Experience with Python (or a similar language) is required. Interest in contributing to the energy transition and to the security of supply. Master's in energy, process, or mechanical engineering, natural science, or related fields, with very good grades
For **project-specific** questions, please **contact**	Supervision team (first supervisors underlined) Dr. B. Pieters, IMD-3, b.pieters@fz-juelich.de Prof. Dr.-Ing. Heidi Heinrichs, ICE-2, h.heinrichs@fz-juelich.de Dr. A. Gerber, IMD-3, a.gerber@fz-juelich.de

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Research Project #23

Impact of ion bombardment on photovoltaic materials (IMD-3 & IFN-1)

Solar cells and modules constitute a fundamental component in the transition towards a sustainable and carbon-neutral energy system, while simultaneously remaining cost-effective. Achieving the 'net-zero emission by 2050' target necessitates an average annual growth of 25% in photovoltaic (PV) energy generation until 2030, culminating in a total installed PV capacity of 5 TW by that year. [1] To facilitate this substantial growth and installed capacity, continuous advancements in the power conversion efficiency of solar cells and modules are imperative. Such improvements are essential not only for further reducing electricity costs, thereby expanding potential applications, but also for mitigating land use conflicts with agricultural or residential areas. Consequently, ongoing research and development of both current and next-generation solar cell materials are crucial.

At present, crystalline silicon solar cells predominate in the market. [2] Among these, architectures utilizing hydrogenated amorphous or nanocrystalline silicon as contact layers, known as silicon heterojunction (SHJ), exhibit the greatest potential for power conversion efficiency. [3] Perovskites have emerged as the most promising next-generation materials, either as independent devices or in conjunction with silicon in a perovskite-silicon tandem (PST) configuration. Both SHJ and PST structures require transparent conducting oxides (TCOs) to facilitate efficient charge carrier extraction and establish low-resistive contact with the metallization. Typically, these TCO materials are deposited via sputtering, a process in which particles ejected from a solid target material bombard the sample, forming a thin film. Regrettably, this process can degrade the SHJ structure or perovskite materials, resulting in reduced device voltages and power conversion efficiencies. While the degradation in SHJ solar cells can be mitigated, perovskites suffer irreversible damage, necessitating an additional protective layer. The precise degradation mechanism remains unclear; however, recent findings suggest that ion bombardment is the primary cause of degradation in both cases. [4-6]

This doctoral thesis seeks to investigate the fundamental mechanisms responsible for sputter process-induced degradation in both SHJ and PST solar cells. Through the strategic design of experiments and the application of diverse simulation tools, this study will further explore the effects of particle bombardment on these photovoltaic materials. By integrating various sputtering techniques, such as radio frequency and direct current, with an understanding of the differing dynamics of generated plasmas, a more comprehensive understanding of the material impacts will be achieved. The findings will be underlined with appropriate simulation results to enhance the understanding of different processes. These external influences on the samples will be correlated with the microstructural properties of the materials under investigation and the observed degradation in device performance. From this analysis, the physical degradation processes will be identified. Ultimately, once the degradation mechanisms are determined, sputter processes will be optimized to mitigate this degradation.

The integration of expertise from the Institute for Energy Materials and Devices – Photovoltaics (IMD-3) and the Institute of Fusion Energy and Nuclear Waste Management – Plasma Physics (IFN-1) facilitates promising opportunities for multifaceted collaboration. IMD-3 contributes extensive knowledge regarding the preparation of materials for photovoltaic applications, their characterization, and prior experience in sputter process-induced degradation. Concurrently, IFN-1 offers in-depth expertise in plasma physics, plasma-matter interaction, and simulation capabilities, alongside advanced experimental and microstructural characterization techniques and facilities, mainly the linear plasma generator PSI-2 [7], where samples can be tested under plasma bombardment with a variety of ions and energies. This collaboration, characterized by complementary knowledge, simulation, and experimental capabilities, is well-positioned to address the complexities of this topic and elucidate various critical aspects of the degradation process.

Key tasks in this project:

- **Detangle different impacts during the sputtering process on perovskite materials:** While for SHJ structures ion bombardment is already identified as main degrading mechanisms, investigations for perovskites are in an earlier phase. Through a proven design of experiments, different impacts during the sputter process should be deconvoluted.
- **Quantify the influence of properties of impinging ion on SHJ structures and perovskites:** Correlate the impact of different ion properties like size/mass, energy or fluency on the degradation effect of the samples under test.
- **Correlate microstructural features of the sample under test with degradation:** Test the extent of degradation on different microstructural features of the samples under test, for example void fraction, hydrogen content or oxygen content in the layers for SHJ structures.
- **Assessing different plasma conditions and their resulting impact on the sample through simulations:** Use advanced simulation models to get insights into plasma dynamics and how particles from the plasma reach the sample. In the following, the impact of the impinging particles on the sample can be simulated and evaluated.
- **Develop a model for the degradation process:** Based on the combined findings from previous tasks, a theory about underlying root causes for the degradation should be developed for the materials under test.
- **Development of degradation-free processes:** Based on the previously generated findings and developed theories, design sputter processes so that they can be applied on SHJ and PST solar cells with minimal degradation.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Materials and Devices - Photovoltaics (IMD-3), Director: Prof. Dr. Christoph Brabec https://www.fz-juelich.de/en/imd/imd-3
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Fusion Energy and Nuclear Waste Management – Plasma Physics (IFN-1), Director: Prof. Dr. Christian Linsmeier https://www.fz-juelich.de/en/ifn/ifn-1
Specific **requirements**	M. Sc. in Electrical Engineering, Materials Science, Physics or comparable Experience in materials science or plasma physics is advantageous
For **project specific** questions please **contact**	Alexander Eberst, IMD-3, a.eberst@fz-juelich.de Dr. Mauricio Gago, IFN-1, m.gago@fz-juelich.de

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Research Project #24

Offline-to-Online Reinforcement Learning for Perovskite Stability Optimization: Benchmarking Against Bayesian Optimization in High-Throughput Experimentation (IMD-3 & JSC)

Research Project Description

Novelty and Innovation:

This project investigates whether reinforcement learning (RL) can outperform established Bayesian optimization (BO) for perovskite stability optimization in high-throughput experimentation. While BO has achieved up to 4x cost-reduction in HTE workflows through exploration-exploitation balancing [1], it suffers from two critical limitations: myopic one-step lookahead potentially leading to local optima, and inability to leverage prior knowledge from publications and thousands of historical experiments worldwide.

Recent breakthroughs in offline reinforcement learning enable training exclusively on historical data (offline) without requiring simulations or new experiments during training [2]. Offline-to-online RL grounds learning in actual experimental data from day one and leverages historic data into optimization policies guiding the experimentation (online). The core scientific question addresses whether RL's theoretical advantages (multi-step planning, long-term strategy learning, implicit prior knowledge integration) translate to practical gains in materials optimization. Through systematic head-to-head benchmarking across three methods (offline RL, pure BO, BO with priors), this work will provide the first rigorous answer defining when, if ever, RL should replace BO for experimental materials science, yielding fundamental insights regardless of outcome.

Main Tasks and Work Packages for the Doctoral Candidate:

- (Month 1 to 6) Establish performance baselines by compiling 5,000+ historical perovskite experiments from IMD-3, and public databases, benchmarking established methods (i.e. pure Bayesian optimization) to quantify current sample efficiency, convergence rates, and limitations in high-dimensional stability optimization.
- (Month 6 to 18) Develop offline-to-online RL framework using Conservative Q-Learning (state-of-the-art offline RL algorithm), training exclusively on historical data without new experiments (JSC infrastructure), developing ensemble surrogate models for uncertainty quantification as safety filters rather than primary simulators, incorporating domain-specific constraints (stoichiometry, temperature, toxicity limits).
- (Month 18 to 30) Perform systematic experimental validation through iterative closed-loop deployment in IMD-3's HTE platform: RL proposes experiment batches → surrogate filtering → human review → HTE execution → policy updates, conducting 200-500 validation experiments across 20-50 cycles, performing comparisons across all methods under identical budgets and conditions with statistical rigor (5 runs/method).
- (Month 30 to 36) Analyze cross-institute transferability and interpretability, testing whether policies trained at IMD-3 transfer to different HTE platforms (at Campus Erlangen), quantifying zero-shot performance and fine-tuning requirements, conducting ablation studies identifying which components contribute most to performance, establishing explainable AI guidelines for when RL provides advantages over BO in different scenarios.

Research Context and Embedding:

Bayesian optimization remains the dominant algorithm for high-throughput experimentation in materials science, yet fundamental questions persist about optimal exploration strategies. Recent work demonstrates two promising directions: offline reinforcement learning enabling learning from historical data without the need for simulations [3], [4], model-based RL [2]. However, no study has rigorously compared RL against BO for experimental materials optimization with real-world validation.

IMD-3 brings critical expertise and resources to this investigation: extensive experience with BO in HTE workflows for photovoltaic materials, measurements on perovskite/OPV stability providing rich datasets for offline RL training and benchmarking studies. A newly built degradation-focused HTE infrastructure at Campus Jülich includes advanced optical perturbation techniques enabling accelerated experimental loops. Most published RL work uses simulated data or limited experimental campaigns, whereas IMD-3's comprehensive historical database provides realistic test cases matching real-world materials research complexity, enabling systematic investigation across composition spaces and prior optimization runs.

The Jülich Supercomputing Center (JSC) provides complementary expertise essential for developing RL algorithms at scale: specialized knowledge in ML and AI development, HPC infrastructure necessary for training RL agents and ensemble surrogate model, established software frameworks for offline RL implementation (Conservative Q-Learning, model-free and model-based approaches). The collaboration enables systematic comparison at scales matching our state-of-the-art autonomous laboratories [5] while maintaining rigorous experimental validation unavailable in purely computational studies.

The research addresses fundamental scientific questions with practical implications for photovoltaic materials development and broader experimental materials science. If RL achieves 2-5x sample efficiency improvement, this enables 2-year stability optimization campaigns completed in 1 year, 50% R&D cost reduction, and instant knowledge transfer between institutions through shared learned policies.

The Graduate School HITEC provides an interdisciplinary community of doctoral researchers working at the intersection of energy materials, AI/ML, and high-performance computing. Since reinforcement learning, autonomous experimentation, and materials informatics are addressed across multiple HITEC specializations, this environment offers valuable opportunities for methodological exchange and cross-disciplinary collaboration in fields of AI, infrastructure and machine-learning.

One step further, beyond photovoltaics the systematic benchmarking framework and offline-to-online RL methodology developed here could transfer to many materials science fields actively investigated at Forschungszentrum Jülich (batteries, hydrogen, catalysis, quantum materials) and is in best accordance with the FZJ strategy to make use of novel Artificial Intelligence methods for experimental acceleration and autonomous discovery platforms. The results will provide a blueprint for offline-online-type problems, and the insights are of high strategic value for the JSC. Beyond energy research, the project learnings will be transferred to other domains, e.g. by the AI consultant team in PI Stefan Kesselheims's lab at JSC.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Materials and Devices - Photovoltaics (IMD-3), Director: Prof. Dr. Christoph Brabec https://www.fz-juelich.de/en/imd/imd-3
Partners of the HITEC Project	Forschungszentrum Jülich, Jülich Supercomputing Centre (JSC), Directors: Prof. Dr. Dr. Thomas Lippert and Prof. Dr. Kristel Michielsen https://www.fz-juelich.de/en/jsc
Specific **requirements**	The candidate has a background in physics, material sciences, electrical engineering, computer sciences
For **project specific** questions please **contact**	Prof. Dr.-Ing. Bugra Turan, IMD-3, b.turan@fz-juelich.de Prof. Dr. Stefan Kesselheim, JSC, s.kesselheim@fz-juelich.de

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Research Project #25

Operando investigation of materials for ammonia cracking (INW-1 & INW-4)

Green ammonia (NH_3) holds significant potential for renewable energy storage and transportation. Due to its high hydrogen capacity, favorable liquefaction properties, and well-established global infrastructure for distribution and handling, it is considered as one of the most promising hydrogen carriers [1-4]. Hydrogen regeneration from ammonia involves an endothermic cracking reaction

$$2NH_3 \quad N_2 + 3H_2 \; \Delta H = 91.2 \text{ kJ/mol}$$

This reaction is typically carried out at high temperatures (> 400 °C) and relatively high pressures (up to tens of bar) [2,3]. It is accelerated using a heterogeneous catalyst (e.g., Ru, Ni, Fe, Co, Fe–Co) [2-4]. An associated challenge is the potential for materials degradation due to nitridation. The harsh cracking environment causes atomic nitrogen to react with the steel surface of the reactor and/or the active components of the catalyst. This may result in restructuring of the material and the formation of undesired nitride layers. Under true reaction conditions, the respective phenomena are challenging to investigate mechanistically. For example, hardly any data for rapid nitridation of steel above 600°C exists [5]. To ensure high performance and longevity of reactors and catalysts, it is essential to gain a comprehensive understanding of these degradation processes.

Towards this end, **this PhD project aims to investigate the atomic scale and microstructural degradation of materials during ammonia cracking through advanced *in situ* and *operando* X-ray characterization techniques**. By employing both surface- and bulk-sensitive X-ray-methods — such as diffraction, reflectometry, spectroscopy, and imaging [6] — we seek to gain detailed **mechanistic insights into material behaviour under true reaction conditions**. Understanding changes in (bulk) structure, surface properties, and oxidation states across scales is essential for optimizing catalysts and reactor materials for the cracking process.

A central focus of the project is to examine the nitridation of reactor walls under reaction conditions, a phenomenon that can accelerate reactor degradation [7]. Various types of steel, including austenitic and high-strength alloys, will be tested. Additionally, the project will explore the effects of the bulk nitridation on the active components of catalysts, investigating both reversible and irreversible structural and surface changes that occur during the cracking process [8]. Catalysts based on Ru, Ni, Co, and Fe will be characterized across different modifications and supports. The *operando* studies of catalyst behaviour under reaction conditions will provide essential information to support the development and testing of promising new catalyst candidates, where nitridation can be suppressed. We expect that we will unravel the time-scales of nitridation and long-term evolution and stability of nitride layers. The insights we gain can guide the proposal and selection of enhanced reactor and catalyst materials for ammonia cracking.

To accomplish these goals, we will use a combination of various complementary X-ray methods to reveal structure, morphology, and chemistry of nitride layers. We will employ sample systems of various complexity, from thin films and steel sheets in gas environment to realistic reactors during operation. A specialized experimental setup will be designed to enable measurements under realistic process conditions, including controlled gas flow and high temperatures and pressures. This setup will be carefully adapted to meet the unique requirements of each characterization technique and will be initially tested using state-of-the art laboratory X-ray machines on model materials such as thin iron films and bulk catalyst crystals. Upon optimization, the setup will be used to conduct experiments on actual reactors and respective realistic components and catalysts. These investigations will also be carried out using international large-scale research facilities, such as synchrotron X-ray sources. These are located for example in Grenoble/France, Hamburg/Germany, Chicago/US, or Stanford/US. This will enable high time resolution and high-throughput investigations under systematically varied conditions to generate large combinatorial data sets, which are analysed using advanced big data analytics and machine learning approaches. The X-ray experiments will be complemented with comparable experiments using neutrons or electrons.

In summary, the PhD project will involve the following key tasks:

- Development of experimental setup for *in situ* X-ray-based characterization during ammonia cracking
- Investigation of reactor steel wall nitridation during reaction conditions (at synchrotron sources)
- Investigation of catalyst nitridation during reaction conditions (at synchrotron sources)
- Analysis and interpretation of experimental data, including big data analytics
- Presentation of research findings at conferences and publication in peer-reviewed scientific journals

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute for a Sustainable Hydrogen Economy - Catalytic Interfaces for Chemical Hydrogen Storage (INW-1), Director: Prof. Dr. Hans-Georg Steinrück https://www.fz-juelich.de/de/inw/unsere-bereiche/inw-1
Partners of the HITEC Project	Forschungszentrum Jülich, Institute for a Sustainable Hydrogen Economy - Process and Plant Engineering for Chemical Hydrogen Storage (INW-4), Director: Prof. Dr. Andreas Peschel https://www.fz-juelich.de/de/inw/unsere-bereiche/inw-4
Specific **requirements**	M.Sc. in Physics, Materials Science, or Chemistry. Experience with structural characterization methods — such as scattering, spectroscopy, or imaging using neutrons, X-rays, or electrons — is highly desirable. Proficiency in data analysis, particularly with Python, is also an advantage.
For **project specific** questions please **contact**	Prof. Dr. Hans-Georg Steinrück, INW-1, h.steinrueck@fz-juelich.de Prof. Dr. Andreas Peschel, INW-4, a.peschel@fz-juelich.de

[1] E. Spatolisano *et al.*: Ammonia as a Carbon-Free Energy Carrier: NH_3 Cracking to H_2. (2023) *Ind. Eng. Chem. Res.* 62 (28), p. 10813.
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Research Project #26

Oxide Thin-Film Catalysts for Chemical Hydrogen Storage (INW-1 & PGI-7)

Efficient, scalable, and safe hydrogen storage remains one of the key challenges for a future hydrogen economy. Liquid Organic Hydrogen Carriers (LOHCs) such as Benzyltoluene or 1,4-Butanediol (BDO) represent an attractive solution due to their high storage density as well as compatibility with existing fuel infrastructure and safe handling characteristics. While there has been significant progress in catalyst design — including Cu-based systems and Pt/TiO_2 for selective LOHC hydrogenation–dehydrogenation [1][2], catalytic cycles for coupling hydrogen separation with storage [3], and metal-exsolution nanoparticle (NP) catalysts for enhanced thermal stability [4, 5]— we posit an urgent need for well-controlled model systems that allow *operando* insight into catalytic mechanisms toward rational materials and process design.

Atomically-defined epitaxial thin films provide unprecedented structural control, enabling the investigation of structure–function relationships at a level that cannot be achieved on powders. When combined with cutting-edge X-ray and electron scattering, spectroscopy, and imaging techniques at INW-1 and PGI-7, these systems offer a unique opportunity to probe catalytic interfaces, NP evolution, and support interactions across length and time scales and under *operando* conditions.

This PhD project will establish oxide thin films as structurally defined model catalysts for hydrogen-storage-relevant reactions, thereby bridging fundamental surface science with applied catalysis in the field of LOHC hydrogenation–dehydrogenation. The overarching goal is to establish epitaxial oxide thin films as a tunable, cross-scale model platform for thermocatalysis in hydrogen-storage reactions.

The PhD student will pursue the following scientific objectives:

Objective 1: Develop and characterize metal-exsolving perovskite thin films as model catalysts

- Grow epitaxial Ni-doped $SrTiO_3$ and related perovskites with controlled doping levels and surface terminations.
- Induce controlled metal exsolution to generate Ni (or alternative) NPs with well-defined size, density, and anchoring geometry.
- Study NP formation, stability, sintering, and re-exsolution under thermal and reactive conditions (BDO dehydrogenation, LOHC cycling).

Objective 2: Establish γ-Al_2O_3 and TiO_2 (anatase) epitaxial thin films as tunable model supports

- Grow γ-alumina thin films to probe acid sites, defect formation, and structure-dependent adsorption of LOHC reactants, intermediates, and products.
- Grow TiO_2 anatase epitaxial films to investigate strong metal–support interactions (SMSI), including Ti migration (“Ti-creep”) onto Pt NPs [5].
- Evaluate how support structure influences catalyst activity, selectivity, and stability.

Objective 3: Determine adsorption geometries, surface structures, reaction pathways under *operando* conditions

- Resolve adsorption geometries of LOHCs and its key intermediates on oxide and metal–oxide surfaces.
- Investigate catalyst surface structure (e.g., NP facets, oxide reconstructions, defect states) during reaction cycles.
- Monitor NP sintering, agglomeration, and dynamic restructuring using *in-situ* and *operando* scattering/spectroscopy/microscopy.

The project combines advanced thin-film growth with cutting-edge X-ray and electron-based techniques to establish epitaxial oxide films as model systems for thermocatalysis. The PhD student will grow high-quality epitaxial γ-Al_2O_3, TiO_2 anatase, and exsolution-active perovskite films using pulsed laser deposition, creating single-crystal-like catalyst surfaces for studying LOHC hydrogenation/dehydrogenation reactions. Structural and morphological evolution will be probed using surface XRD, CTR, and XRR, while GISAXS/GIWAXS will track NP nucleation and sintering under reaction conditions. Chemical and electronic changes will be monitored with near-ambient pressure XPS, complemented by depth-resolved XAS (TEY/TFY) and nanoscale-resolved XPEEM to capture lateral heterogeneity and metal-support interactions.

Catalytic behavior will be assessed through temperature-programmed and controlled hydrogenation/dehydrogenation experiments, enabling direct correlation of structural dynamics with catalytic function. The project will deliver a tunable model platform capable of revealing fundamental mechanisms in hydrogen-storage-relevant catalysts, offering insight into interface restructuring, defect chemistry, nanoparticle evolution, and reactions such as selective BDO dehydrogenation and reversible LOHC cycling. These results will inform rational catalyst design for hydrogen separation, storage, and release, with relevance across thermocatalysis and industrial hydrogen technologies.

The PhD student will work within the combined expertise of INW-1 and PGI-7 at Forschungszentrum Jülich: INW-1 provides leading *operando* X-ray capabilities and catalytic interface science, while PGI-7 offers world-class epitaxial thin-film growth infrastructure, including the Electronic Oxide Cluster for integrated PLD–XPS–XPEEM studies. Additional collaborations with ESRF and PETRA III as well as LOHC and exsolution research groups ensure a highly interdisciplinary environment. The student will receive comprehensive training in thin-film growth, advanced scattering, spectroscopy and imaging, catalysis, and data analysis, forming a strong foundation for a career in energy materials or hydrogen technologies.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute for a Sustainable Hydrogen Economy - Catalytic Interfaces for Chemical Hydrogen Storage (INW-1), Director: Prof. Dr. Hans-Georg Steinrück https://www.fz-juelich.de/de/inw/unsere-bereiche/inw-1
Partners of the HITEC Project	Forschungszentrum Jülich, Peter Grünberg Institute – Electronic Materials (PGI-7), Director: Prof. Dr. Regina Dittmann https://www.fz-juelich.de/en/pgi/pgi-7
Specific **requirements**	M.Sc. in Physics, Materials Science, or Chemistry. Experience with structural characterization methods — such as scattering, spectroscopy, or imaging using neutrons, X-rays, or electrons — is highly desirable. Proficiency in data analysis, particularly with Python, is also an advantage.
For **project specific** questions please **contact**	Dr. Peter Walter, INW-1, p.walter@fz-juelich.de Dr. Felix Gunkel, PGI-7, f.gunkel@fz-juelich.de

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