

# Atomistic Modelling of Solid-Liquid Interfaces in Electrocatalysis

8 - 12 January 2024 / Lorentz Center@Oort

## Science

This workshop aimed to tackle the complexity of electrode-electrolyte interfaces for relevant applications in electrocatalysis by bringing together physicists, chemists, electrochemists, materials scientists, and engineers with complementary expertise in computational modelling of: (i) solid surfaces and solid-liquid interfaces; (ii) complex liquid phases (dielectric solutions); (iii) electrocatalysis and (iv) machine learning. The focus of the event was to discuss the state-of-the-art and beyond in the development of approaches and methods for the accurate modelling of electrochemical processes. Some of the biggest challenges in the field, that we aimed at addressing during the workshop were:

- 1) Improvement of implicit solvation models,
- 2) The inclusion of the explicit liquid phase in the simulations
- 3) Study of the effect of the electrolyte solution on the catalysis
- 4) The inclusion of an external applied potential

These aspects are important to achieve an accurate, quantitative description of electrochemical processes which can be directly correlated with experimental investigations.

The discussions revolved around bridging gaps in knowledge related to electrolyte structure, ion interactions, and the impact of an applied potential on reaction mechanisms. A holistic approach would be needed to capture the intricacies of electrocatalysis and move towards a more realistic representation of the electrochemical environment. The workshop recognized the potential of machine learning (ML) in advancing computational electrocatalysis. The integration of ML algorithms, including non-local descriptors, was identified as a promising avenue for improving the efficiency and accuracy of simulations, representing a leap forward in computational capabilities.

The realization that many challenges in computational electrocatalysis are shared among researchers has created a sense of unity. Identifying common obstacles allowed participants to combine each other's expertise and propose innovative solutions collectively. The shared experience deepened the sense of community among workshop attendees. Networking opportunities during coffee breaks and poster sessions reinforced the idea that building a scientific community is essential to address the challenges discussed during the workshop.

A notable tangible outcome is the commitment to write a commentary paper on the workshop's topic. Participants aim to contribute to a high-impact factor journal, providing a comprehensive overview of the workshop's discussions, insights, and proposed solutions. This tangible outcome reinforces the workshop's impact and ensures the broader dissemination of its findings within the scientific community.

The workshop facilitated meaningful discussions, resulting in tangible outcomes such as the establishment of new connections, potential collaborations, and a more robust network of professionals in the computational electrocatalysis community. To build on this collaborative spirit, participants have expressed the intention to submit a COST Action proposal, envisioning a platform for sustained collaboration and knowledge exchange.

## Organization & Format

The workshop on "Atomistic Modelling of Solid-Liquid Interfaces in Electrocatalysis" employed a meticulously crafted format aimed at encouraging collaborative discussions, facilitating interdisciplinary exchange, and addressing the challenges within computational electrocatalysis. In preparation for the workshop, surveys were distributed to participants, focusing on challenges and future directions in computational electrocatalysis. The results of these surveys were analyzed and discussed on the first day of the workshop. The insights gained from the surveys were instrumental in shaping the subsequent discussions and setting the stage for the brainstorming sessions.

The workshop spanned five days, with each day dedicated to addressing a specific challenge in the field. Morning sessions featured expert speakers who provided foundational insights into each day's theme. Afternoons were dedicated to open discussions and brainstorming sessions, where participants were divided into sub-groups to discuss specific challenges highlighted by the survey. The dynamic composition of these sub-groups changed daily, promoting cross-fertilization of ideas. This format facilitated active participation, ensuring that all attendees had an opportunity to contribute their insights, fostering a sense of shared ownership of the workshop's objectives. The workshop dedicated a session to young researchers, providing them with a platform for poster presentations.

The success of the workshop was not only attributed to the engaging scientific program but also to the impeccable organization and support provided by the Lorentz Center. The quality of facilities, logistics, and accommodation was excellent, contributing significantly to the overall positive experience of all participants. The seamless coordination and thoughtful arrangements enhanced the collaborative atmosphere, allowing participants to focus on the scientific discussions. As organizers, we extend our gratitude to the Lorentz Center and eagerly anticipate future opportunities to host events in such a conducive and professionally managed environment.

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