universität wien
Department of Functional Materials and Catalysis
Institut für Funktionelle Materialien und Katalyse

Materials Workshop
Mini-Symposium

When: 27.03.2026, 14:00-17:00 Uhr

Where: Kleiner Hörsaal 3 / HS3, Halbstock, Boltzmanngasse 1

Host: Assoz. Prof. Jia Min Chin, PhD

1) Prof. Christian Schröder: Ionic liquids as electrolytes: A molecular perspective

Ionic liquids have emerged as promising electrolytes for electrochemical energy technologies, owing to their high thermal stability, wide electrochemical windows, and exceptional chemical tunability. At the same time, their use challenges many concepts derived from conventional dilute electrolytes, as ionic liquids exhibit strong ion–ion correlations, pronounced local structuring, and complex transport and reactive behavior.

In this introductory lecture, I provide a molecular-level perspective on ionic liquids as electrolytes, aimed at an audience without prior background in molecular simulations. After introducing the basic characteristics of ionic liquids and their relevance for batteries, fuel cells, and electrolyzers, I discuss how their structure, dynamics, solvation properties, and polarization effects govern ionic and proton transport as well as electrochemical reactivity. Particular emphasis is placed on the behavior of ionic liquids at electrochemical interfaces, where molecular organization and charge redistribution play a decisive role for device performance.

The lecture highlights why many of these phenomena are difficult or impossible to access experimentally and why molecular simulations are indispensable for developing a mechanistic understanding. Without entering methodological details, the talk establishes the physical and chemical concepts needed to appreciate modern simulation approaches. In this way, it sets the stage for the subsequent lectures on machine-learning-based interatomic potentials and on the simulation of electron and proton transfer processes in advanced electrolytes and at electrochemical interfaces.

Short Bio: Prof. Christian Schröder (Universität Wien)

Prof. Christian Schröder is a full University Professor in the Institute of Computational Biological Chemistry at the University of Vienna. He serves as Deputy Head of the institute and is a member of the editorial board of the European Society on Ionic Matters.

He studied chemistry in Giessen and Göttingen in Germany and completed his PhD at the Max-Planck Institute of Biophysical Chemistry in Göttingen on vibrational energy transfer. After postdoctoral work on protein-water interfaces, he joined the University of Vienna, where he progressed from university assistant to full professor, habilitating on computational studies of molecular ionic liquids.

Prof. Schröder's research focuses on molecular simulation and theoretical studies of solvation dynamics, ionic liquids, and computational spectroscopy, often employing advanced molecular dynamics methods and polarizable force fields. His work spans fundamental physical chemistry and applications to complex liquids and biomolecular systems.

2) Prof. Luis Miguel Varela: Simulation of energy storage materials: Applications to solid electrolytes interfaces and proton transfer

Electron and proton transfer processes are fundamental to the operation of electrochemical devices such as batteries, fuel cells, and electrolyzers. A proper understanding and optimizing electron and proton transport is essential for advancing sustainable energy technologies, which usually demand computer simulations to circumvent highly sophisticated and even impossible experimental observations. In this talk we review several applications performed in our research group of different simulation techniques (molecular dynamic simulations, specifically those based on neural network potentials, and DFT-based methods to the simulations of electron and proton transfer processes through electrolytes (water-in-salt, ionic liquids) and at the electrochemical interface with relevant electrode materials to mimic redox reactions such as the formation and growth of the solid electrolyte interface, and hydrogen or oxygen evolution reaction mechanisms in electrolyzers and fuel cells.

Short bio: Luis Miguel Varela (University of Santiago de Compostela)

Luis Miguel Varela (Lugo, 1972) graduated in Physics at the University of Santiago in 1995 and in Law at the Open University (UNED) in 2000. He got his PhD in Physics (with Honors) from the University of Santiago de Compostela, where he is currently full professor in its department of Particle Physics (Condensed Matter division). His teaching has focused on thermodynamics, statistical mechanics, and statistical data analysis, as well as on Econophysics and on the thermodynamics of Renewable Energies.

His research interests focus on the statistical mechanics of complex systems, especially complex charged fluids, and more specifically on ionic liquids, and on complex networks and their applications in epidemics, socioeconomic systems, interregional development, etc. Specifically, it works on the properties of ionic fluids and ionogels as advanced electrolytes for the storage of electrochemical and electrical energy (batteries, supercapacitors, fuel cells, electrolyzer membranes...), and as active media in photonic devices. He has also made contributions in the field of thermal energy storage and thermal fluids. He is the author or co-author of more than 160 articles, chapters, and monographs in these fields, and more than 120 conference communications, having directed 14 doctoral theses and more than forty graduate and master's theses, and coordinated regional, national, and European projects, as well as such as research contracts with industries and with the Public Administration. In addition, he is the inventor of several patents in the field of energy harvesting devices and materials for energy applications. Currently, it has active research and teaching collaborations with researchers from different universities and research centers, including Cambridge, Oxford, Sorbonne, Vienna, Milan,

Marburg, Göteborg, Helmholtz Institute of Münster, Porto or Naples, among others. He has acted as visiting professor at Sorbonne Université and Universitá degli Studi di Milano Bicocca.

He has been Dean of the Faculty of Physics at the University of Santiago de Compostela from 2010 to 2018 and has coordinated its Master's in Physics and Master's in Renewable Energies and Energy Sustainability programs at USC, as well as its Doctoral program in Renewable Energies and Energy Sustainability. He has also coordinated the Galician network of Ionic Liquids and is founding president of the European Society of Ionic Matter (www.web-esim.eu), which integrates researchers from different universities and national and European research centers.

3) Hadrian Montes-Campos: Simulation of energy storage materials: Reactive Machine Learning Interatomic Potentials

Understanding and improving materials for energy storage requires tools that can describe how atoms interact, move, and sometimes react. Traditional computational models are often either too simplified to capture complex chemistry or too expensive for large-scale simulations. Machine-learning interatomic potentials offer a promising alternative, combining high accuracy with computational efficiency.

In this talk, I will introduce the basic ideas behind neural-network-based interatomic potentials, explaining how they learn atomic interactions from quantum-mechanical data. I will then present examples of their application to energy-related materials, focusing on ionic liquids as advanced electrolytes. In particular, I will show how reactive machine-learning models enable the study of polarisation effects, proton transfer, and structure–dynamics relationships in these complex fluids.

These approaches open new possibilities for the predictive design of next-generation materials for electrochemical energy storage.

Short bio: Hadrián Montes-Campos (University of Santiago de Compostela)

Hadrián Montes-Campos is a Postdoctoral Researcher at the University of Santiago de Compostela (Spain), working at the interface of computational physics, electrochemistry, and machine learning. He obtained his PhD in Materials Science in 2021 with highest distinction and the Extraordinary PhD Award, after completing his MSc and BSc in Physics at the same institution.

His research focuses on the theoretical and computational design of advanced electrolytes for sustainable energy technologies, including ionic liquids, nanoconfined systems, and hydrogen-related materials. He is the developer of *NeuralIL*, one of the first differentiable neural-network force fields specifically designed for ionic liquids and charged fluids, enabling quantum-accurate simulations of reactive and polarisation effects at realistic scales.

Dr. Montes-Campos has authored 39 peer-reviewed publications and has delivered invited and keynote lectures at major international conferences. His work combines molecular dynamics, density functional theory, and machine-learning interatomic potentials to advance predictive modelling of electrochemical interfaces and proton-conducting media. He currently leads

machine-learning developments within national and European projects and serves as Secretary of the European Society of Ionic Matter (ESIM).

His long-term research goal is to establish next-generation ML-driven simulation frameworks capable of bridging atomistic modelling and materials design for energy storage and green hydrogen technologies.