Bio

Prof. Michael Eikerling received his Ph.D. in Physics from Technische Universität München (TUM) in 1999. From 2003 to 2019, he was Professor of theoretical chemical physics and electrochemical materials science at Simon Fraser University in Burnaby, British Columbia, Canada. Between 2003 and 2013, he held a cross-appointment to the fuel cell institute of the National Research Council of Canada in Vancouver, BC, where he shaped a program in physical modeling of fuel cells. As of May 2019, he was appointed as Professor at RWTH Aachen University and inaugural Director at the new subinstitute for Modeling and Simulation of Materials in Energy Technology (IEK-13) within Forschungszentrum Jülich, Germany. His research employs a comprehensive spectrum of methods in physical theory and computation, to approach a diverse range of scientific challenges, from fundamental to applied topics. Vital activities focus on transport phenomena at interfaces and in nanopores, theory and computation of electrocatalytic phenomena, self-organization in electrochemical materials, statistical physics of heterogeneous media, porous electrode theory, and modeling and diagnostics of electrochemical devices. He has published over 140 journal articles (h-index 37) and 1 book. In 2017, Michael Eikerling was awarded the Alexander Kuznetsov Prize for Theoretical Electrochemistry of the International Society of Electrochemistry, in recognition of his groundbreaking work on modeling polymer electrolyte fuel cells, with an emphasis on water management, transport and electrocatalysis. He serves on editorial boards of Scientific Reports and Electrocatalysis and engages strongly in affairs of the international electrochemical community.

Abstract

Deciphering Electrocatalytic Reactions with Theory and Computation

The growing demand for highly efficient and environmentally benign energy technologies drives research on electrochemical materials. In this realm, theory, modeling, and simulation are contributing increasingly powerful methods and tools to study how complex multifunctional materials come to life during self-organization, how they live and work, and how they age and fail. The grand challenge of theoretical electrocatalysis is to unravel the functional relationship between the electrode potential and net conversion rates of reactions of interest, such as the oxygen reduction, oxygen evolution, or CO₂ reduction reaction. A major goal in this field is to develop a self-consistent computational approach that is based on first principles and accurately represents sensitivities of reaction mechanisms, pathways, and rates to the composition and structure of electrocatalyst materials, thermodynamic state of the electrode-electrolyte interface, and local reaction conditions. The seminar will give a critical account of approaches being developed in this field, viz. address their capabilities and current limitations. Thereafter, it will present a theoretical framework that integrates DFT-based calculations of reaction energetics, a
theoretical interface model, and a microkinetic model of reaction kinetics. Capabilities of this approach in view of generating mechanistic understanding, facilitating materials selection and design, and yielding effective kinetic parameters for electrode modeling will be discussed.