NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE

MSE's 30th Anniversary Colloquium Series

Data-Enhanced Multiscale Theory of Operando Energy Conversion Systems

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Abstract

Emerging operando spectroscopies and microscopies reveal a highly dynamic behavior of interfaces in energy conversion systems. Insufficient insight and the concomitant inability to control or exploit the corresponding strong structural and compositional modifications centrally limits the development of performance catalysts, electrolyzers or batteries required for a sustainable energy supply for our society. Predictive-quality modeling and simulation has become a major contributor to accelerated design all across the materials sciences, not least through powerful computational screening approaches. Current first-principles based methodology is nevertheless essentially unable to address the substantial, complex and continuous morphological transitions at working interfaces. I will review this context from the perspective of first-principles based multiscale modeling, highlighting that the fusion with modern machine learning approaches is likely key to tackle the true complexity of working systems. Approaches pursued by our group thereby aim at maximum data efficiency by exploiting physical models wherever possible or through active learning that only queries data on demand. Illustrative examples will be drawn from thermal methanation catalysis, electrocatalytic oxygen evolution and organic semiconductor photovoltaics.

Biography

Prof. Karsten Reuter's research activities focus on a quantitative modeling of materials properties and functions. He specifically works on multiscale models that combine predictive-quality first-principles techniques with coarse-grained methodologies and machine learning to achieve microscopic insight into the processes in working catalysts and energy conversion devices. Karsten did his doctoral studies on theoretical surface physics in Erlangen, Madrid and Milwaukee. Following research experiences at the Fritz Haber Institute of the Max Planck Society (MPG) in Berlin and the FOM Institute in Amsterdam, he headed an independent MPG junior research group. From 2009 to 2020, he was Chair for Theoretical Chemistry at the Technical University of Munich (TUM) and has been appointed as director of the Theory Department of the Fritz Haber Institute in 2020. He recently held visiting professorships at Stanford (2014), MIT (2018), and Imperial College London (2019). He is also the coordinator of the Munich Cluster of Excellence e-conversion, and acting chair of the Surface Science Division of the German Physical Society.

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Live streaming via: https://ntu-sg.zoom.us/w/92534897666

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