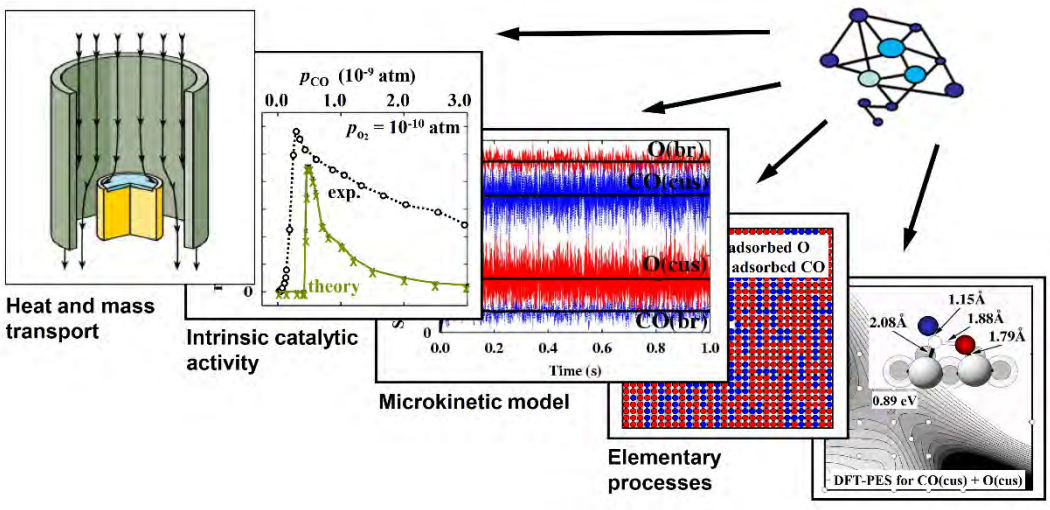
Physikalisches Kolloquium des Fachbereich Physik
Arnimallee 14, D-14195 Berlin
Freitag, 08. Januar 2021, 15 h s.t., Online-Veranstaltung

MERGING MULTISCALE THEORY AND DATA SCIENCES TO TACKLE OPERANDO ENERGY CONVERSION SYSTEMS

Karsten Reuter, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany, reuter@fhi-berlin.mpg.de

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 [1], 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 [2], electrocatalytic oxygen evolution [3] and organic semiconductor photovoltaics [4].



References

[1] A. Bruix, J.T. Margraf, M. Andersen, and K. Reuter, Nature Catal. **2**, 659 (2019).
[2] M. Deimel, K. Reuter, and M. Andersen, ACS Catal. **10**, 13729 (2020).
[3] J. Timmermann, F. Kraushofer, N. Resch, Z. Mao, M. Riva, Y. Lee, C. Staacke, M. Schmid, C. Scheurer, G. Parkinson, U. Diebold, and K. Reuter, Phys. Rev. Lett. **125**, 206101 (2020).
[4] C. Kunkel, C. Schober, J.T. Margraf, K. Reuter, and H. Oberhofer, Chem. Mater. **31**, 969 (2019).