Hamburg Photon Science Colloquium

MULTISCALE THEORY FOR OPERANDO ENERGY CONVERSION SYSTEMS

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Emerging operando spectroscopies and microscopies reveal a highly dynamic behavior of interfaces in working energy conversion systems. In catalytic systems, this involves continuous reaction-induced (surface) morphological transitions or even a liquid-like behavior. I will review this context from the perspective of first-principles based multiscale modeling, highlighting that modern machine learning approaches are likely key to tackle the true complexity.

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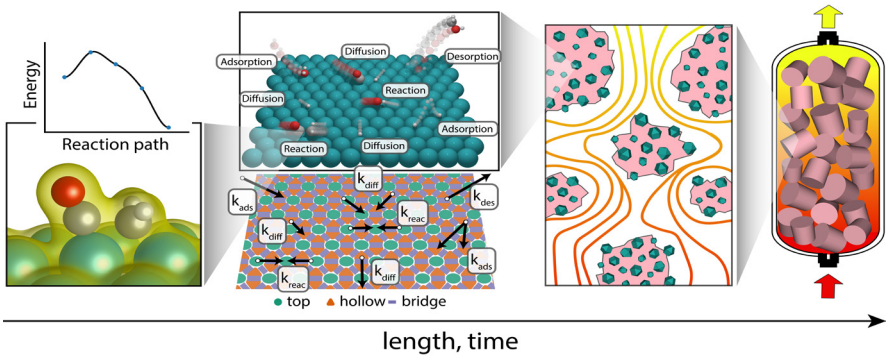
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