



Stéphane Kenmoe. Foto: Vladimir Unkovic

The authors explain that modern science rests on three well-established pillars: the classic categories of experiment and theory and the younger computer simulation methods, with big data science rapidly becoming a fourth. While current experimental techniques have recently advanced their time and space resolution, dynamic atomistic computer simulations struggle to reach increasingly long time and length scales.

Two good friends?

Interactions between experiments and molecular dynamics simulations

By Stéphane Kenmoe and Eckhard Spohr

‘Experiment is the only means of knowledge at our disposal. Everything else is poetry, imagination.’ This famous quotation is around one hundred years old and comes from the German physicist Max Planck, who won the Nobel prize in 1918 for his discovery of energy quanta. If Planck came back to life today, he would be surprised at how things have progressed. He was certainly far from imagining the revolution that his own and his contemporaries’ work would spawn. Indeed, with the advent of quantum theory and the invention of the transistor and the computer, theory, and its numer-

ical realization in high performance computers, has become a powerful and indispensable tool of scientific research, which was not even conceivable at his time.

Introduction

At the time one of us started his scientific career in the 1980s, atomistic computer simulation was an emerging technology, which rapidly expanded its scope from its original field of application – the statistical mechanics of liquids – to the atomistic description of almost any kind of material and the molecular

description of processes in biology on ever-expanding length and time scales. The influential book *Computer Simulation of Liquids*¹ presented graphics that have since become iconic and that depicted computer simulation as the third pillar of science, separate to theory and experiment. At present, this three-pillar basis of modern science is once more about to be enhanced, as data science is considered by many to be yet another pillar in its own right.

Atomistic computer simulation methodology is often interpreted as experiment’s (numerical) theory and theory’s (numerical) computer

experiment. This Janus-like nature derives from the fact that computer simulation is, at its very heart, a method to generate (representative) members of a statistical mechanical ensemble, based on a (Hamiltonian) model that describes the interactions between atoms and molecules. In the following, the term ‘atomistic simulation’ should be taken in the narrow sense that ground state properties of the system (at 0 K) are not sufficient or appropriate for the problem of interest, but rather dynamical and statistical aspects of the system must be taken into account at finite temperature. As long as computational resources are finite (they always will be!), atomistic simulations involve a trade-off between shortcomings in the description of the nature of the interactions (approximating the ‘Hamiltonian’ to various degrees) and shortcomings due to the incompleteness of the set of representative microscopic states (‘configurations’) of the ensemble – insufficient sampling of phase space or ‘bad statistics’, as it is often termed. While steady progress has been made in both regards over the last few decades, the central problem still persists: finding the proper balance between these two shortcomings. This problem will not go away, as all progress in computer hardware, simulation software, and methodological advances will be swallowed by the requirements of ever-increasing system sizes and ever-increasing time scales of processes, and even the nature of processes – i.e. whether they can be described by essentially a classical picture or whether they require the use of quantum mechanics.

In the following, we plan to offer our personal view on what is a fruitful and promising path to interaction between dynamic atomistic computer simulation and experiment. We will base this to some extent on our recent experience within the framework of the Collaborative Research Centre/Transregio 247 (CRC/TRR 247) ‘Heterogeneous Oxidation



(1) The magnitUDE HPC system of UDE, the work horse for many research groups. Source: Image taken from https://www.uni-due.de/css/magnitude_main.php

Catalysis in the Liquid Phase’. The systems of interest are intrinsically complex and involve:

- More than a single phase
- Electron transfer
- Proton transfer
- ‘Static’ heterogeneity: dopant and impurity atoms may be important, while alloys and mixed oxides can be random or stoichiometric
- Surface segregation, i.e. inhomogeneous phases
- Dynamic heterogeneity: during a catalytic cycle, the structure of the working catalyst (*in operando*) may change on much longer time scales than those on which the *chemical* reaction occurs
- Open thermodynamic systems
- Electronically excited states: spectroscopy, photo(electro)chemistry
- Issues of spin multiplicity, magnetism etc.
- Boundary conditions that cannot generally be implemented in a straightforward way for a Hamiltonian system within the dynamic framework of Newton’s or Schrödinger’s (or any more advanced set of) equations of motions

- ... and many more.

The practical merits and (simultaneously) the limitations of dynamic atomistic computer simulations are, in our view, predominantly the following:

- The value of computer simulations lies mostly in generating insight by answering questions of the type ‘*what if...?*’ rather than ‘*how large...?*’.
- Due to the fact that system sizes and observation lengths are so limited in practice, simulations must be staged, i.e. one needs specific ideas about the nature, composition and geometric setup of the system (which can come only from experiment) to even start.
- The many necessary approximations and the limited experimental resolution *in situ* and *in operando* limit the merit of single simulations in most cases; instead, a (possibly large) number of simulations employing different structural assumptions of the system, or variants of a single one, are needed in order to test the role of the ‘known’ unknowns in these assumptions as much as possible.

- The insight gained by dynamic simulations is very much *time-dependent*, in the sense that with advances in hardware, software, theory and algorithms every few years the insight changes, often *qualitatively*, and certainly *quantitatively*.

Individual simulations may well take months to complete or, rather, to be terminated at a – whatever the term means – *reasonable level of statistical accuracy*. This requires tremendous computing resources, which need to be financed, installed, managed, and kept secure (UDE’s *magnitUDE* high performance computing (HPC) system was inaccessible for several months of 2020 as a consequence of a pan-European attack on HPC systems), ranging from individual group clusters to university resources (see Fig. 1) and national and international HPC institutions.

Insight, not (only) numbers

Oxides, in particular non-noble metal oxides, are the most abundant surface substrates in the accessible part of the Earth, and many attempts have recently been made to harness their properties for energy and for catalytic research. Such oxides interact strongly and in a complex way with water, which gives rise to many detrimental corrosive processes on the one hand, but also renders the surface of these materials sufficiently mobile and atomically heterogeneous to allow chemical reactions that would otherwise not be possible on the other hand. On the atomic level, this local mobility stems from local proton transfer processes that allow for the dynamic formation and destruction of surface OH bonds originating from oxygen atoms that bridge metal atoms on the oxide surface. Thus, while during an oxidation reaction the electrons can be transferred (and consumed) by changing the valency of the metal atoms, the proton transfer that is usually coupled (at least when oxidizing

organic compounds) can be assisted by temporarily changing the protonation state of oxygen-containing local species or groups in the oxide or in the aqueous solution. In addition, the unique solvation properties of water allow for the solvation and transport of promotor atoms (or, in general, ‘catalytic impurities’) from the environment and along the oxide surface. This all produces an amazing structural and dynamic heterogeneity at the site of an oxidation reaction, which makes the very chemical question concerning the mechanism of a relatively simple chemical reaction (in other words, insight into this reaction) a fascinating and challenging one. This insight, at least for us, is one of the many worthwhile goals of CRC/TRR 247.

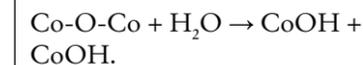
Can we model this complexity and heterogeneity using dynamic atomistic simulations? The quick answer is ‘No!’, at least not quantitatively, but what we can do is model several aspects. Taking Co_3O_4 as an example: among many other indirect insights concerning the local reactivity of various faces, edges, and corners of nanoparticles of different sizes, experimental evidence shows that so-called A- and B-terminated (001) surfaces (which differ in the cobalt/oxygen ratio of the ideal clean surface) exhibit different activities towards several catalytic reactions. Furthermore, many experimental setups (at high temperature and high pressure) provide little structural information about local water content on the surface.

We have thus chosen to model this issue by comparing idealized periodically extended surfaces of A- and B-terminated (001) Co_3O_4 surfaces, covered by between one and two water molecules per cobalt atom in a given layer [T. Kox et al., *Front. Energy Res.*, 8, 604799, 2020]. The A-terminated free cobalt oxide surface reconstructs (undergoes a structural change), which happens on many surfaces in order to maximize coordination numbers of atoms near the surface. The first

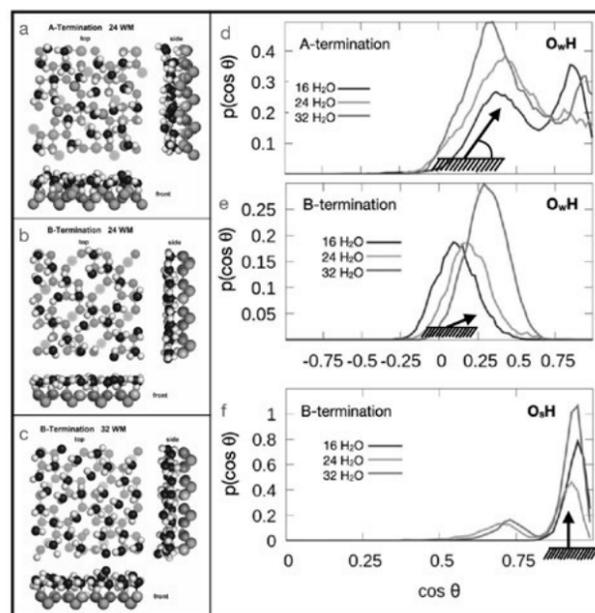
observation of interest that we made was that the reconstruction is lifted in the presence of water and that this is due to the fact that oxygen atoms originating from adsorbed water molecules contribute to the increase of coordination number in such a way that the driving force for reconstruction is reduced.

Figure (2) shows a subset of data from a series of such simulations for a water coverage of 1.5 water molecules per cobalt atom (in a single layer, altogether 24 water molecules) for A-termination (Fig. 2a) and B-termination (Fig. 2b) as well as for 2 water molecules (altogether 32 water molecules) for B-termination (Fig. 2c). A and B-termination differ in the fact that a half-layer of Co^{2+} ions is located on top of the topmost oxygen layer (green atoms, not all of which are shown in the central part of Fig. 2a). Note that at intermediate water content the water molecules on the B-terminated surface (2b) appear to be more ordered than on A-termination (2a), and that, furthermore, the hydrogen atoms on the B-terminated surface appear to be located approximately at the same height from the surface (side view) as the oxygen atoms, whereas many hydrogen atoms point towards the vacuum on the A-terminated surface. At higher water content (2c), the B-terminated surface also exhibits a number of dangling OH bonds.

These differences in behaviour can be shown to be the consequence of (or at least correlated with) the distinctly different numbers of OH groups that are produced on the different surfaces by splitting a bridging metal-oxygen-metal bond and simultaneously dissociating a water molecule on the surface according to the net reaction



The resulting structures, the number of such OH groups, and the dynamical nature of these bonds that form and break during the simula-



(2) Left: snapshots with top (centre), front (below) and side views (right) of simulations with 1.5 water molecules per layer for A-termination (a) and B-termination (b) and with 2 water molecules per layer and B-termination (c). Right: distributions of the orientation of OH bond vectors of hydroxy groups with oxygen atoms from water molecules for A-termination (d) and B-Termination (e) and for OH groups with oxygen from cobalt oxide lattice (f).

Source: T. Kox, S. Kenmoe, E. Spohr, in preparation.

tion would be difficult to predict from static electronic structure calculations that, however, might have the benefit of an improved description of the electronic interactions in the system (e.g. by replacing approximate quantum mechanical density functional theory with more accurate wave function-based electronic structure theory). We would like to note that several other projects within the CRC/TRR 247 (projects A5, B4, and B8 by the groups of Hättig, Pentcheva, Manganas/Neese and Schmid) study exactly these *complementary* aspects. This illustrates the conflict between *accuracy* on the one hand (our results may or may not be relevant, since the detailed atomic nature of the system may or may not be the one we staged in the simulation) and the necessary *statistical requirements* to actually observe the phenomenon itself.

The observation that hydrogen atoms ‘stick out’ of some surfaces and not of others is associated with

the fact that the orientation of the various OH groups (water OH bonds and surface OH groups) changes with surface conditions and is by no means uniform and static (as one might expect at very low temperature). In fact, the surface exhibits both *static and dynamic heterogeneity*. The structural inhomogeneity is visible on the right side of Figure (2). Here, the distributions of the cosine of the angle between the OH vector and the surface normal are shown. Typical orientations are shown inside the graphs. The first thing to note is that the distributions are more or less broad. No single prevalent structure exists. Second, there are systematic differences between A-termination and B-termination, resulting from the different valency and local environments of cobalt atoms near the surface. With increasing water content, systematic changes can be observed that originate from the increasing importance of hydrogen-bonding interactions,

at the expense of the importance of surface interactions. Finally, it may be interesting to point out an obvious fact: over the simulation time of about 20 ps, the OH groups with oxygen from water (d and e) are clearly different from the OH groups with oxygen from the cobalt oxide surface. This is an indication of the vastly different time scales for hydrogen motion (hydrogen atoms are quite mobile) and oxygen motion (oxygen atoms from the lattice do not exchange with oxygen atoms in the liquid over the simulated time period). Finally, one can also observe for the higher water content simulations on the B-terminated surface (f) that subtle structural changes on the surface apparently give rise to a new subspecies of OH groups that are tilted and obviously engaged in hydrogen bonding with the water layer.

One may ask oneself: what do these subtle structural changes have to do with catalysis? Frankly, we don’t know! But one can reasonably safely extrapolate, based on the fact that very many different local environments exist already on (out of computational necessity) idealized two-dimensionally flat interfaces, that even more such environments will exist on a real catalyst consisting of nanoparticles with many different facets, edges, and corners or an irregularly nanostructured surface with kinks, ridges, point defects, etc. Some of these environments, which fluctuate around local quasi-equilibrium structures and evolve and shift over longer time scales, may well become important in activating a reactive event. Since, even in a good catalyst, the characteristic turn-over time (mean time between two reactions at the same ‘site’), is many orders of magnitude longer than the time for reactions itself (of the order of femtoseconds to picoseconds), such fluctuations or evolutions are very likely to be relevant in some (unknown) way. Experimentally, this issue is addressed by various attempts at in *operando* studies of

various probe properties. Such studies are usually highly limited by their spatial and temporal resolution, which often leads to the unfortunate fact that most of the measured signal originates from the ‘catalyst at rest’ rather than from the ‘working catalyst’. While experiment usually has a lower practical limit on accessible time and length scales, computer simulation methods, as pointed out before, usually exhibit an upper practical limit of time and length scales. Experiment and simulation are continuously progressing to – eventually – meet. At present, we are exploiting the data underlying our understanding of solvent effects, fluctuations and disorder to compare it with experimental imaging techniques, like TEM, STM, or AFM, and local spectroscopic probes, such as SFG, in frequent exchange with the experimental groups working in A4, B5 and B7 of CRC/TRR 247.

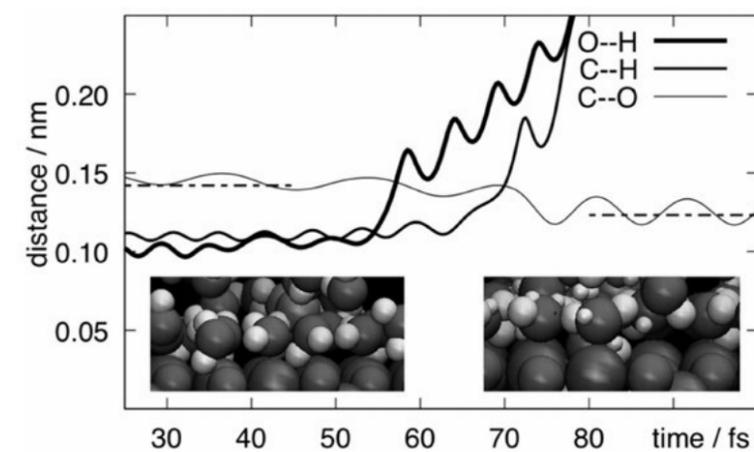
The average orientation of the various OH groups, together with the polarization of the solid oxide, gives rise to and determines the interfacial electrostatic potential drop, which is an important quantity that determines the electrochemical properties of this interface. In principle, it is known how one can calculate the electrochemical potential of such an interface, at least for very basic choices of complexity. However, doing this in a sound way according to the rules of statistical mechanics, requires orders of magnitude of larger computational efforts, and the result would nevertheless depend very much on *how the simulation was staged*. Valiant efforts in this direction have recently been made by Sprik et al.² and others, who have established the theory on how to do this, and who have used computer simulations as the experimental tool to prove the viability of their theoretical concepts. In our work, we prefer to look at the other Janus face of computer simulations, namely as experiment’s numerical theory tool, to investigate the

microscopic consequences beyond what experiments can currently resolve in terms of length and time scales.

Simulations often live on stage, rarely in the wild

While it is *difficult to determine the precise value* of the interfacial potential in a straightforward manner, one can *easily change the interfacial potential* and thus the driving force for oxidation reactions in computer simulations (but in an ill-defined way) by applying a simple computational trick: although the simulations discussed above contain a certain number of water molecules, the simulation methodology does not prohibit the inclusion of additional hydrogen atoms (or oxygen atoms) or the removal of some of the water hydrogen atoms. It is obvious that in a hydrogen-deficient system the driving force for the oxidation of a 2-propanol molecule will increase (it is just not easy to know how much), so that one can investigate, for instance, the influence of the interfacial and hydration environment on the oxidation of solvated alcohols, such as 2-propanol, which is studied intensely within CRC/TRR 247.

Figure 3 shows the time dependence of the alcohol O-H distance, the C-H distance at the central carbon atom and the hydrogen atom bonded to it, and the C-O distance from a simulation where 8 hydrogen atoms have been removed. The insets show the differences in water orientation between the unperturbed reference (left), which shows more hydrogen atoms close to the surface, and the hydrogen-poor system (right), where almost no hydrogen atoms point towards the surface. The graph shows that the oxidation reaction is initiated at around 55 fs by a proton transfer from the more acidic hydroxy hydrogen (fat line). After this proton has been fully transferred to a neighbouring oxygen atom (at around 65 fs) the C-H bond widens, and at around 70 fs the C-O bond reacts to the changed environment and becomes shorter, as is to be expected when the C=O double bond in acetone is formed. The dash-dotted lines indicate the equilibrium distances of the initial C-O single bond (around 0.142 nm; left) and of the final C=O double bond (around 0.122 nm; right). While the two hydrogen atoms diffuse away from the acetone molecule attached to water molecules, the excess reac-



(3) Time dependence of the OH, CH and CO distances in a reactive simulation of 2-propanol. The insets show snapshots of simulations of the unperturbed reference system (left) and a modified system where eight hydrogen atoms are removed. Source: A.M. Omranpoor, E. Spohr, S. Kenmoe, in preparation

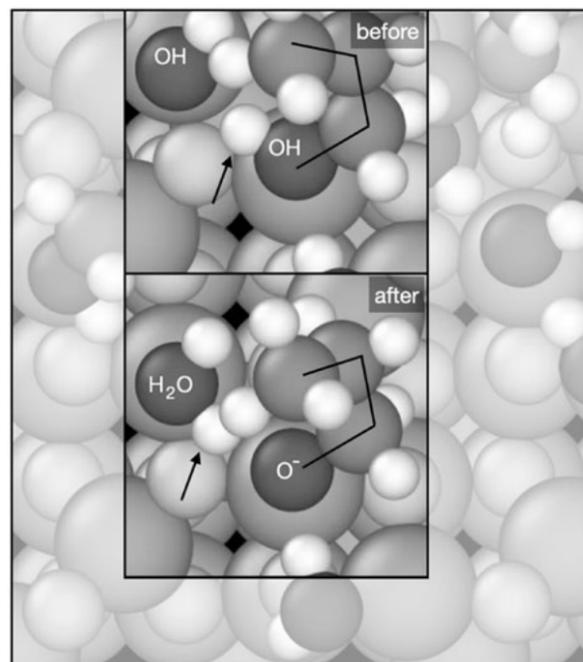
tion energy, which is (partially) deposited in the C=O bond, has not yet decayed on the depicted time scale, as can be seen by the relatively large amplitude of oscillation.

Don't start from scratch; compare!

Insight is usually generated in small incremental steps. Scientific revolutions are rare events, just like chemical reactions. Having studied the cobalt oxide/water interface in detail, we now turn to the cobalt ferrite/water interface, the oxide that is most obviously the focus of research activities in CRC/TRR 247, and we analyse and *compare* the local structural changes. Not only is the range of local environments larger near the CoFe_2O_4 than near the Co_3O_4 surface, but, in addition, the consequences of Jahn-Teller distortion effects in the ferrite have to be addressed, which has hampered recent progress in the calculations. Without being able to compare the ferrite system to the more 'well-behaved' Co_3O_4 case, based on the first results one might have speculated about some interesting, or rather surprising, properties in the ferrite case³.

Another goal of our project is to study the effect of defects and single dopants, with the goal in mind of comparing the local environments with TEM images, generated *in situ* or *ex situ*, of relevant (or seemingly interesting) local arrangements (project B7). While it is possible to address specific properties, such as band gaps or other spectroscopic properties, given the limited range of dopant concentrations (here, simulations can usually only model rather large concentrations because of the small total number of particles), it is impossible to learn much about the doped system without comparing the changes in electronic and optical properties to the structural changes relative to the parent material.

In yet another subproject, we are currently addressing the elemen-



(4) Snapshot from a simulation of a mixture of co-adsorbed 1-propanol and water on a Co_3O_4 surface with B-termination after proton transfer from the alcohol to an adsorbed hydroxy group. The top inset shows the original state before proton transfer.

Source: A.M. Omranpoor, E. Spohr, S. Kenmoe, in preparation

tary steps of alcohol oxidation on Co_3O_4 by comparing simulations of single 1-propanol molecules (solvated in an aqueous film) with monolayers and mixed layers of 1-propanol (see Fig. 4). The goal here is to compare the observed structural features with results from SFG experiments in project B5. Since, experimentally, the exact composition of the interfacial layer to which the experiment is sensitive is not known, a variation of different 'what if' scenarios can prove helpful for the interpretation of the experiments. The figure shows, for a system containing coadsorbed water and 1-propanol molecules, a first proton transfer step from the acidic OH group of 1-propanol to a water-originating adsorbed OH group (O_w in Fig. 2), forming an intermediate water molecule. While this step might be the first stage of an oxidation reaction, the resulting alcoholate ion in this particular case is only transiently stable and reacts back after a few femtoseconds to a state similar to that labelled 'before'.

The time dependence of computer simulation-generated insight

Many of the insights gained by computer simulations in chemistry are time dependent, in the sense that, on the one hand, the simulation methodology (Hamiltonian model and boundary conditions) changes over time and, on the other hand, the details of what forms the relevant aspects of reality are based on changing experimental evidence and detail, which forms the underlying assumptions that must be made in order to stage the simulated system. An example of the former is brought about by the irresistible shift from empirical force field simulations to simulations based on quantum mechanical density functional theory (DFT). One of us (ES) was quite active in modelling structure, dynamics and aspects of chemical reactivity at the metal/water interface using – by necessity – classical force field models to describe the relevant aspects of interactions.

However, a fundamental aspect that is important to understand the frequently studied platinum/water interface, namely the underpotential deposition of hydrogen, was impossible to model at the time. With the advent of DFT, such calculations become possible, rendering many of these early results somewhat obsolete. Nevertheless, some insight survived. It was recognized early on that configurational entropy at finite temperature is an important aspect of the interface, leading to continuous orientational distributions of molecular orientations near idealized surfaces, different in detail, but not dissimilar to those in Figure (2). In this context, it is interesting to realize the considerable time it takes for computer simulation-generated insight to enter textbooks: by now many, but not all, electrochemistry textbooks have switched from simple Ising-type dipole-up/dipole-down models towards continuous models when describing the important role of the aqueous side of the liquid/solid interface in electrochemistry.

It is a foregone conclusion that due to theoretical and statistical mechanical progress, DFT-based simulations will also only provide transient insight. Obviously, spectroscopic and spin-dependent properties on the transition metal oxide surface and, in general, any non-adiabatic effects require, in order to produce insight, more than only ground state properties as delivered by DFT. Thus, another round of methodology-inspired changes of insight into these problems is already on the horizon.

While waiting for this, one can imagine that in the very short term experimental and simulation-generated views coalesce towards a coherent view of the atomistic details of material structure and dynamics. Very much in the spirit of Richard Feynman's inspirational lecture 'There's plenty of room at the bottom', nanostructured materials offer a realistic perspective for experiment and simulation merging at a

common length scale: while hardware and methodological advances allow simulating increasingly large systems, for increasingly long times, with more phenomena included in the system description (thereby advancing to the *top* of computational abilities), experiments at the same time become increasingly focused on local events, at increasingly short times, thus advancing to Feynman's bottom.

However, reality is complex: time and length scales do not (yet?) match, experiments are possible but often not precise enough, simulations do not (or cannot) use the adequate theoretical framework, both experiments and simulations take too long to set up and to execute. Nevertheless, one should 'always look on the bright side'. Perhaps data science will be able to overcome the present impasse if it can advance beyond its present focus on establishing correlations towards providing causality. If all these endeavours work perfectly, and eventually they will, the cross-fertilization of experiment, simulation and theory will produce *true imagination transfer*, in analogy to the underlying processes of electron and proton transfer in oxidation catalysis at the interface between transition metal oxides and the aqueous liquid state.

Summary

Modern science rests on three well-established pillars: the classic categories of experiment and theory and the younger computer simulation methods, with big data science rapidly becoming a fourth. While current experimental techniques have recently advanced their time and space resolution, dynamic atomistic computer simulations struggle to reach increasingly long time and length scales. Within CRC/TRR 247 we strive to reach common scales for experiments and simulations for the case of alcohol oxidation reactions

on transition metal interfaces in contact with aqueous solutions. Here, we describe some of our recent results concerning the structure and dynamics of cobalt oxide interfaces and the role of the aqueous environment for the oxidation of 1-propanol and 2-propanol. We show in a qualitative fashion how the role of the environment leads to structural heterogeneity near the interface, for increasing water content and for increasingly oxygen-rich environments. The discussion proceeds in the light of the shortcomings and strengths of dynamic atomistic computer simulations. These are rooted in the facts that simulations of such complex systems, like the one studied here, need experimental input to start, that results are very strongly model dependent and often more qualitative than quantitative in nature, and that the comparison between similar simulations is an important means to contribute to qualitative understanding and insight into the processes underlying oxidation catalysis in the liquid state.

Die moderne Wissenschaft ruht auf drei etablierten Säulen: den klassischen Kategorien von Experiment und Theorie und den jüngeren Computersimulationsmethoden, wobei Big Data Science schnell zu einer vierten wird. Während aktuelle experimentelle Techniken in letzter Zeit ihre Zeit- und Ortsauflösung verbessert haben, arbeiten dynamische atomistische Computersimulationen damit, immer größere Zeit- und Längenskalen zu erreichen. Innerhalb des CRC/TRR 247 bemühen wir uns, gemeinsame Skalen für Experimente und Simulationen für den Fall von Alkoholoxidationsreaktionen an Übergangsmetall-Grenzflächen in Kontakt mit wässrigen Lösungen zu erreichen. Hier beschreiben wir einige unserer jüngsten Ergebnisse bezüglich der Struktur und Dynamik von Kobaltoxid-Grenzflächen und



Eckhard Spohr. Foto: Vladimir Unkovic

der Rolle der wässrigen Umgebung für die Oxidation von 1-Propanol und 2-Propanol. Wir zeigen qualitativ, wie die Rolle der Umgebung zu struktureller Heterogenität in der Nähe der Grenzfläche führt, und zwar für zunehmenden Wassergehalt und für zunehmend sauerstoffreiche Umgebungen. Die Diskussion erfolgt vor dem Hintergrund der Unzulänglichkeiten und Stärken von dynamischen atomistischen Computersimulationen. Diese wurzeln in dem Umstand, dass Simulationen solcher komplexer Systeme wie dem hier untersuchten, zu Beginn experimentellen Input benötigen, dass die Ergebnisse sehr stark modellabhängig und oft eher qualitativer als quantitativer Natur sind, und dass der Vergleich zwischen ähnlichen Simulationen ein wichtiges Mittel ist, um zum qualitativen Verständnis und zur Einsicht in die der Oxidationskatalyse im flüssigen Zustand zugrundeliegenden Prozesse beizutragen.

Annotations/Literature

- 1) M. P. Allen and D. J. Tildesley, Oxford University Press, New York, 1987
- 2) C. Zhang and M. Sprik, Phys. Rev. B, 94, 245309 (2016)
- 3) T. Kox, S. Kenmoe, E. Spohr, in preparation

The authors

Stéphane Kenmoe is a research scientist and project coordinator at the University of Duisburg-Essen, Germany. He was born in Ngaoundere, Cameroon. His graduate studies at the University of Dschang, also in Cameroon, enabled him to obtain a master's degree in condensed matter physics. He then spent one year at the International Centre for Theoretical Physics (ICTP) in Trieste, Italy. In 2011, he undertook a PhD in theoretical physico-chemistry at the Max Planck Institute for Iron Research in Düsseldorf, Germany, which he obtained in 2015. He is currently working on interactions between water and nanoparticles to better understand how they can facilitate the production of energy. Stéphane Kenmoe is also a science popularizer on TV and social media. He is a science writer and novelist, as well as a science movie producer and actor. He is also very active in networking for the promotion of early career scientists, for whom

he initiated the CASESMA prize, a regional award to encourage young scientists in the field of computational physical chemistry. He is an event organizer for capacity building (schools, conferences, workshops...) and for connecting science and society through the project 'Making Science the Star' of which he is the promoter. He has won several awards, among which the recent diversity prize for academic leadership at the University of Duisburg-Essen in Germany.

Eckhard Spohr studied chemistry at Johannes Gutenberg University Mainz and at the University of California, Irvine. He finished his diploma in 1983 and obtained his PhD in 1986 at the Johannes Gutenberg University Mainz. Subsequently, he was a research associate at the Max Planck Institute for Chemistry in Mainz until 1988. This was followed by a postdoctoral Feodor Lynen Research Fellowship from the Alexander von Humboldt Foundation in the Department of Chemistry and the Institute for Surface and Interface Science at the University of California, Irvine. From 1991 to 2000, he was a research associate in the Institute of Theoretical Chemistry at Ulm University, where he finished his habilitation in 1995. This was followed by a two-year period as a research associate at the Institute for Energy Research at the Forschungszentrum Jülich, before he became head of the research group 'Fundamentals of the Physical Chemistry of Fuel Cells'. Since 2007, he has been a professor of theoretical chemistry at the University of Duisburg-Essen. He was awarded the Otto Hahn Medal by the Max Planck Society in 1988 and the Merckle Research Prize by Ulm University in 1998.

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DOI: 10.17185/duepublico/75363

URN: urn:nbn:de:hbz:464-20220128-134021-7

Published in: UNIKATE 57 (2021), p. 123-132

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