

COST Action 18234: Virtual Mobility Grant Report

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1 Introduction

The continued combustion of fossil fuels to satisfy a growing energy demand have led the world to the brink of a climate crisis. Instead of transferring carbon from the lithosphere into the atmosphere to obtain our energy, we must re-cycle elements already present in the atmosphere or biosphere, i.e., C, H, O, and N, to produce recyclable carriers for renewable energy. Closing the associated water and CO₂ cycles will be among the key enablers for this grand challenge, as this holds the key to converting energy to synthetic fuels.

Abundant molecules such as water and CO₂ are the ideal feedstock for the chemical storage of energy created from renewable sources. Two potential routes are splitting water into O₂ and H₂, and converting CO₂ into higher-value products. The most-promising conversion processes are Electrocatalysis and Photocatalysis, but low turnover efficiencies and the need for precious metal catalysts are the primary factors preventing widespread adoption. We need to replace rare with abundant elements or at least reduce their amounts, or discover alternative, inexpensive catalysts with high activity, selectivity, and stability.

Unfortunately, simulating the catalytic reactions required to tackle these goals challenges current theoretical methods. Density functional theory, the workhorse of modern electronic structure theory, does not well capture the details of charge transfer processes involved in catalytic bond dissociation or formation. The multi-scale nature of catalytic reactors spans many scales - from the atomistic picture of individual charge transfer processes to larger-scale questions regarding the chemical engineering of reactor conditions. Many multi-scale models have been proposed to solve this challenging multi-scale problem. Indeed, modeling catalysis attracts scientists from many different fields with their own methods, expertises and requirements in terms of accuracy or speed. Given the large number of subtly different theoretical schemes, it is useful to categorize these approaches and identify properties such as areas of expertise, available methods, their ranges and limitations, as well as use cases and points of contact. The present document contains a first collection of methods, developed and used by members of COST action 18234. To this end, we set up and evaluated a form sent out to the action participants. In the following we present the results. This compendium will hopefully prove useful to scientists working in or entering this community as it will help identify areas of intersections, current challenges and deficiencies. The main goal is not to provide exhaustive descriptions, but rather a brief overview of available tools and methods, and points of contact to obtain additional information. If you feel you can add to this list, please contact florian.libisch@tuwien.ac.at with a brief description of the method you use, its limitations, a few references and a point of contact.

2 Experts who have replied to this survey (as of April 2024)

We list those members of CA 18234 and associated researchers that answered our survey, providing a point of contact and their general areas of expertise. We will keep updating this document based on new submissions. Our action covers a wide range of expertise, from the atomistic scale of ab-initio modeling to large-scale approaches.

1. Hristiyan Aleksandrov, Faculty of Chemistry and Pharmacy, Sofia University, Bulgaria, investigates a wide range of materials at different scales from complexes of transition metal ions, metal nanoparticles, porous materials and small clusters to metal surfaces.
2. Anja Bieberle-Hütter, DIFFER, the Netherlands, focuses in her research on experiments and modeling of materials for the energy transition. Her aim is to identify the limitations at electrochemical interfaces to provide important information to design improved catalysts and structures. From the experimental side, her research interests are on thin film deposition and microstructuring of metal and metal oxide thin films, as well as their chemical, structural, spectroscopic and (photo-)electrochemical characterization. In modeling and simulation, Anja Bieberle-Hütter focuses mainly on **microkinetic modeling**, including bridging to other length

scales and by this doing **multi-scale modeling**. Bieberle-Hütter employs custom code for microkinetic modelling.

3. Sofia Calero, Eindhoven University of Technology, the Netherlands, develops simulations for renewable energies and energy efficiency, including the development of force fields, algorithms and simulation methods to reverse engineer the properties of materials. One of the hallmarks of her research is bridging the gap between computational physics-chemistry and industry. An important part of her research activity is carried out in close collaboration with large and small industries that benefit from the knowledge and scientific transfers that her group develops. Together, using advanced simulation techniques, they are successfully unraveling many mechanisms involving multifunctional nanostructured materials. In her calculations, Calero uses an in-house developed Molecular Dynamics (MD) (MD) and Monte Carlo techniques code, RASPA, and iRASPA for visualization.
4. Maytal Caspary Toroker, the Helen Diller Quantum Center, Technion, Israel, investigates energy materials. She has developed a method for charge transport calculation through heterostructures using **wave propagation**. She has also conducted research on transition metal oxides for their applications as photocatalysts and photoelectrodes. She developed a method to calculate the band edge positions using ab-initio approaches. These band edge positions play a crucial role in determining the suitability of these materials for various applications. Apart from this, she also works on metal organic frameworks (MOFs) and covalent organic frameworks (COFs) for their application in photocatalysis and electrocatalysis.
5. Nigel Clarke, the University of Sheffield, UK, studies theoretical polymer and soft matter physics, as well as the rheology of polymers and gels. These materials require **computational modeling at the mesoscale**, including techniques such as **drift diffusion models** and **kinetic Monte Carlo**, which are implemented in a custom code.
6. José R. B. Gomes, CICECO, University of Aveiro, Portugal, uses computers and computational methods in chemistry and in materials science to investigate catalysis. He employs several different computational techniques (Density functional theory, molecular mechanics (MM), QM/MM, force fields and molecular dynamics (MD) or coarse-grained (CG) simulations, docking, 3D-QSAR, microkinetic modelling) to analyze the interactions and reactions of adsorbates (in gaseous or in solution) with materials or enzymes.
7. Anders Hellman, Chalmers competence centre for Catalysis, Sweden. His research interests include surface science and heterogeneous catalysis, gas-surface interactions, hot-electron chemistry, electron-hole excitations. Employed methods include **density-functional theory**, **Monte-Carlo techniques**, and Micro-kinetic models models. Hellman uses PyCatKin for kinetic calculations of catalytic reactions.
8. Eugene Kotomin, Institute of Solid State Physics, University of Latvia, Latvia, simulates defects in solids, with ab initio and semi-empirical calculations of the electronic structure of perfect insulating crystals, surfaces and defects, with mechanisms of defect creation under irradiation, defect diffusion, and recombination, with the kinetics of bimolecular and tunnelling reactions. These problems of Defect modeling relate to both theoretical condensed matter physics and chemical physics of insulating solids, as well as to theoretical quantum chemistry of non-metallic crystals with special emphasis on the materials science aspects.
9. Florian Libisch, Institute for Theoretical Physics, TU Wien, Austria, is a theoretical solid state physicist who aims at multiscale descriptions of nanodevices and catalytic processes. He combines density functional theory with large-scale **tight binding** approaches to achieve quantum-mechanical descriptions at larger scales. Embedding methods methods allow for the accurate descriptions of **charge transfer processes** at surfaces. Libisch employs custom tight-binding and transport codes. The embedding method is available from E. A. Carter.

10. Sergei Piskunov, Institute of Solid State Physics, University of Latvia, Latvia, develops methods for computer simulations of materials and processes. In the context of CA 18234, he performs quantum-chemical simulations of chemical reactions in different environments and near surfaces of solids to describe catalysis.
11. Dorota Rutkowska-Żbik, Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish academy of sciences, Poland, investigates oxidative dehydrogenation of light alkanes, activation of small organic molecules, biomass valorisation: conversion of furfural and furfurool, as well as catalytic oxide-based materials used to synthesise high added-value products for energy and polymer applications. She uses Density Functional Theory (DFT) as well as Time-Dependent Density Functional Theory (TD-DFT) to investigate metal complexes and metal-containing heterogeneous catalysts.
12. Bartek Szyja, Wrocław University of Science and Technology, Poland, investigates theoretical aspects of catalysis, including **surface** and **chemical reactivity**, **photocatalysis** and **electrocatalysis**. In particular, he develops methods to handle **charge transfers**, zeolite synthesis, Employed methods include **Density functional theory**, **multiscale modelling approaches** and **ReaxFF force-field** parametrizations. Force fields are implemented in GULP, forcematching is done by Szyja inhouse. Atomic population is analysed with Chargemol.
13. Vesselin Tonchev, Institute of Physical Chemistry, Bulgarian Academy of Sciences, Bulgaria, develops methods for Cellular Automata, including **transfer matrix approaches**, solving ODE-systems, and **scaling analysis**. Tonchev uses custom code for these tasks.
14. Péter Vancsó is a computational solid-state physics with direct relevance to nanoelectronics. In close collaboration with experimentalists, he is working on novel two-dimensional materials investigating their physical properties and their future potential for catalytic and electronic applications. He uses standard electronic structure and theoretical solid state methods like density functional theory or MD simulations, as well as methods for evaluating transport properties. Vancsó has custom Tight-Binding, Transport and Hubbard codes and uses available software for DFT and MF.
15. Titus van Erp, Norwegian University of Science and Technology, Norway, investigates the simulation of chemical processes at large time- and length scales. Simulating important processes in biological or industrial processes require crude approximations or invoking uncertain assumptions. His research aims to bring forward the molecular understanding of complex processes using state-of-the-art simulation techniques. This includes the development of new innovative methodologies that can enhance the accuracy of present methods and expand accessible time- and system scales of computer simulations. Key methodologies include (ab initio) Molecular Dynamics (MD), **Monte Carlo** methods, **path sampling** and **rare event sampling**. van Erp's group develops code for path sampling and rare event molecular simulations (PyRETIS and InfinityRETIS).

3 Use cases related to water splitting

In this section we note the use cases participants provided which relate to the aim of Cost Action 18234, the problem of water splitting, and list references when provided. We also present the abstracts of some of these publications.

1. Thermal dissociation of water and the electrochemical CO oxidation.
Abstract of "The determining role of T_x species in the catalytic potential of MXenes: Water adsorption and dissociation on Mo_2CT_x ", Gouveia and Gomes [2023]: "Density functional theory is used to investigate the origins of the excellent catalytic activity of the Mo_2CT_x MXene

for the water gas shift reaction. By considering different possibilities for the MXene surface termination ($T_x = \text{none, O, F, or a mixture of O and F}$), we conclude that its ideal composition should contain both F and O adatoms, essential for controlling the exothermicity of the reaction and avoiding saturation by oxygenated species. More precisely, while Mo_2CO_2 and Mo_2CF_2 are too inert towards water adsorption and dissociation and the bare Mo_2C MXene is inactivated upon coverage by oxygenated species, our calculations predict that regions near one or two O adatoms in the midst of F surface terminations should be the active catalytic sites. Indeed, in the vicinity of the O adatoms, water adsorbs with moderate strength, dissociates with a very low energy barrier (0.14–0.20 eV), and the dissociation is moderately exothermic.”

2. Photostimulated water splitting.

Abstract of "Photocatalytic water splitting of improved strontium titanate for simultaneous separation of H_2 in a twin photoreactor", Tai et al. [2023]:

"A core-shell structural Rh-CrO_x loaded on Al³⁺ doped strontium titanate was used for photocatalytic water splitting. A specially designed twin photoreactor, which integrates the water splitting and the degradation of isopropanol, can simultaneously carry out the degradation of isopropanol and hydrogen production. A flux method was conducted to prepare Rh@CrO₃ cocatalyst on Al³⁺ doped high-crystallinity strontium titanate for the photocatalyst of hydrogen evolution. Nearly 1200 $\mu\text{mole/g}$ of hydrogen was evolved in photocatalytic whole water splitting in five hours under simulated AM 1.5 G sunlight. Pt-loaded WO₃ was utilized to degrade 100 ppm isopropanol solution. The above photocatalysts were used in the twin reactor with electron-mediator I^-/IO_3^- and a Neosepta anion-exchanged membrane. Hydrogen evolution of 1102 $\mu\text{mole/g}$ and isopropanol removal of 10.1% were achieved in five hours, indicating the rate-limiting H_2 rate was overcome. The quantum efficiencies on the hydrogen-evolution and degradation sides were estimated to be 0.102% and 0.123%, respectively."

3. Simulation of the electrochemical interface of water splitting; particular focus on OER by microkinetic modeling; use of DFT to estimate rate constants. (Samanta et al. [2022], George et al. [2019a, 2020], Liang et al. [2021b], George et al. [2019b], Liang et al. [2019], Zhang and Bieberle-Hütter [2016], Zhang et al. [2016], Kishore et al. [2019], Liang et al. [2022])

Abstract of "Understanding the Impact of Different Types of Surface States on Photoelectrochemical Water Oxidation: A Microkinetic Modeling Approach", George et al. [2020]:

"The oxygen evolution reaction (OER) has been identified as one of the performance-limiting processes in solar water splitting using photoelectrochemical (PEC) cells. One of the reasons for the low OER performance is related to the existence of different types of surface states at the semiconductor–electrolyte interface: recombining surface states (r-SS) and surface states due to intermediate species (i-SS). Since the impact of surface states on OER is still under debate, we investigate how different types of surface states affect PEC water oxidation and how they impact experimental measurements. In a new computational approach, we combine a microkinetic model of the OER on the semiconductor surface with the charge carrier dynamics within the semiconductor. The impact of r-SS and i-SS on the current–voltage curves, hole flux, surface state capacitance, Mott–Schottky plots, and chopped light measurements is systematically investigated. It is found that (a) r-SS results in a capacitance peak below the OER onset potential, while i-SS results in a capacitance peak around the onset potential; (b) r-SS leads to an increase in the OER onset potential and a decrease in the saturation current density; (c) r-SS leads to Fermi-level pinning before the onset potential, while i-SS does not result in Fermi-level pinning; and (d) a smaller capacitance peak of i-SS can be an indication of the lower catalytic performance of the semiconductor surface. Our approach in combination with experimental comparison allows distinguishing the impact of r-SS and i-SS in PEC experiments. We conclude that r-SS reduces the OER performance and i-SS mediates the OER."

4. AIMD water dissociation (Moqadam et al. [2018]) via path sampling (RETIS algorithm). Improved algorithm reducing wall time from 1 year to 10 days (Zhang et al. [2024]). In addition

demonstrations of the simulation technique to protein folding and water boiling phase transition.

Abstract of "Highly parallelizable path sampling with minimal rejections using asynchronous replica exchange and infinite swaps", Zhang et al. [2024]:

"Capturing rare yet pivotal events poses a significant challenge for molecular simulations. Path sampling provides a unique approach to tackle this issue without altering the potential energy landscape or dynamics, enabling recovery of both thermodynamic and kinetic information. However, despite its exponential acceleration compared to standard molecular dynamics, generating numerous trajectories can still require a long time. By harnessing our recent algorithmic innovations—particularly subtrajectory moves with high acceptance, coupled with asynchronous replica exchange featuring infinite swaps—we establish a highly parallelizable and rapidly converging path sampling protocol, compatible with diverse high-performance computing architectures. We demonstrate our approach on the liquid–vapor phase transition in superheated water, the unfolding of the chignolin protein, and water dissociation. The latter, performed at the ab initio level, achieves comparable statistical accuracy within days, in contrast to a previous study requiring over a year."

5. Investigation of the role of the charge transfers between the system components in redox-catalysis.

Abstract of "Ru-pincer complexes as charge transfer mediators in electrocatalytic CO₂ reduction", Szyja et al. [2024]:

"In this work, we unravel the role of the system components in the charge transfer processes occurring in the 2-electron reduction of CO₂. We focus our analysis on the pincer-complex/graphene composite system in order to explain the role of the donors of the pincer ligands in the elementary charge transfer processes. To achieve this goal, we have used the unique combination of the constrained DFT method and computational hydrogen electrode. The results obtained this way allowed us to conclude that the catalytic performance of the system depends to a great extent on the electron-donating properties of the Ru-pincer complex. We have determined, that the optimal charge transfer in the system is due to the easy, single-step transfer to the activated CO₂ molecule and the energies required for such transfer are comparable to the limiting potential of the reaction."

6. The influence of surface doping on catalytic properties of water-splitting catalysts. (Dymkowski et al. [2023], Szyja and Podsiadły-Paszowska [2020], Podsiadły-Paszowska et al. [2019])

Abstract of "Helping Thy Neighbor: How Cobalt Doping Alters the Electrocatalytic Properties of Hematite", Szyja and Podsiadły-Paszowska [2020]:

"We present analysis of the indirect role of Co doping on the electrocatalytic activity of α -Fe₂O₃. Upon substitution of one of the Fe atoms in the hematite surface, we observed a promoting effect of the substitution, upon which the overpotential required for the water-splitting reaction decreased in all substitution sites investigated. The cobalt site itself, however, does not exhibit the improved properties with respect to the undoped hematite. The promoting effect results purely from the altering of the properties of the nearest Fe atoms in the hematite surface. We conclude that the overpotential is reduced upon formation of the structure resembling the O₂ molecule strongly interacting with the surface between the Co and Fe sites, and this is consistent with the catalytic activity of the surface vacancies of the hematite."

7. Descriptors for bonding and electronic structure in the context of catalytic processes. (Podsiadły-Paszowska et al. [2019], Kizior et al. [2023])

Abstract of "Partial Methane Oxidation to Methanol on Ru-Porphyrins – on the Role of Non-Innocent Ligands and Spin Crossover", Kizior et al. [2023]:

"The partial oxidation reaction of CH₄ led to the formation of CH₃OH in the presence of Ru-porphyrin oxo complexes (denoted as POR, POR-O and POR-OH where in the case of the last two, oxygen atom and the OH group were attached to the active site, respectively), in

which Ru was present on different oxidation states. The simulations were performed based on Density Functional Theory (DFT) with extended geometric and electronic structure analyses of each reaction step. Moreover, the reaction pathways were investigated in different spin states. The Spin Crossover (SCO) phenomenon was found to play an important role in the kinetics of the reaction in the presence of POR and POR-O. Harmonic Oscillator Model of Aromaticity (HOMA) index was applied for different spin states to estimate the aromaticity changes of the pyrrole rings in the Ru-porphyrin complexes. In order to characterize the nature of bonding, the Natural Bond Orbitals (NBO) analysis including the Wiberg Bond Index (WBI) and Natural Population Analysis (NPA) was carried out. Finally, the Non-Covalent Interactions (NCI) index was employed to gain insight into interactions between the components of the reaction. It was found that the non-covalent interactions cannot be neglected in the studied reaction paths.”

8. Dissociative adsorption of Oxygen on Aluminum: use of embedding methods to accurately treat charge transfer.

Fragment of Abstract of "Embedded Correlated Wavefunction Schemes: Theory and Applications", Libisch et al. [2014]:

"In this Account, we review embedded correlated wavefunction (CW) approaches and some applications. We first discuss our density functional embedding theory, which is formally exact. We show how to determine the embedding potential, which replaces the interaction between subsystems, at the DFT level. CW calculations are performed using a fixed embedding potential, that is, a non-self-consistent embedding scheme. We demonstrate this embedding theory for two challenging electron transfer phenomena: (1) initial oxidation of an aluminum surface and (2) hot-electron-mediated dissociation of hydrogen molecules on a gold surface. In both cases, the interaction between gas molecules and metal surfaces were treated by sophisticated CW techniques, with the remainder of the extended metal surface being treated by DFT. Our embedding approach overcomes the limitations of conventional Kohn–Sham DFT in describing charge transfer, multiconfigurational character, and excited states. From these embedding simulations, we gained important insights into fundamental processes that are crucial aspects of fuel cell catalysis (i.e., O₂ reduction at metal surfaces) and plasmon-mediated photocatalysis by metal nanoparticles. Moreover, our findings agree very well with experimental observations, while offering new views into the chemistry. We finally discuss our recently formulated potential-functional embedding theory that provides a seamless, first-principles way to include back-action onto the environment from the embedded region."

9. Transition metals in zeolites and biological systems - DFT studies on preferred sitting and catalytic properties.(Kornas et al. [2023], Oszejca et al. [2023], Porebska et al. [2023], Orzeł et al. [2024])

Abstract of "Unraveling the Molecular Mechanism of S-Nitrosation Mediated by N-Acetylmicroperoxidase-11", Oszejca et al. [2023]:

"Conversion of NO to stable S-nitrosothiols is perceived as a biologically important strategy of NO storage and a signal transduction mechanism. Transition-metal ions and metalloproteins are competent electron acceptors that may promote the formation of S-nitrosothiols from NO. We selected N-acetylmicroperoxidase (AcMP-11), a model of protein heme centers, to study NO incorporation to three biologically relevant thiols (glutathione, cysteine, and N-acetylcysteine). The efficient formation of S-nitrosothiols under anaerobic conditions was confirmed with spectrofluorimetric and electrochemical assays. AcMP-11-assisted incorporation of NO to thiols occurs via an intermediate characterized as an N-coordinated S-nitrosothiol, (AcMP-11)Fe²⁺(N(O)SR), which is efficiently converted to (AcMP-11)Fe²⁺(NO) in the presence of NO excess. Two possible mechanisms of S-nitrosothiol formation at the heme-iron were considered: a nucleophilic attack on (AcMP-11)Fe²⁺(NO⁺) by a thiolate and a reaction of (AcMP-11)Fe³⁺(RS) with NO. Kinetic studies, performed under anaerobic conditions, revealed that the reversible formation of (AcMP-11)Fe²⁺(N(O)SR) occurs in a reaction of RS⁻ with (AcMP-11)Fe²⁺(NO⁺) and ex-

cluded the second mechanism, indicating that the formation of $(\text{AcMP-11})\text{Fe}^{3+}(\text{RS})$ is a dead-end equilibrium. Theoretical calculations revealed that N-coordination of RSNO to iron, forming $(\text{AcMP-11})\text{Fe}^{2+}(\text{N}(\text{O})\text{SR})$, shortens the S–N bond and increases the complex stability compared to S-coordination. Our work unravels the molecular mechanism of heme-iron-assisted interconversion of NO and low-molecular-weight thiols to S-nitrosothiols and recognizes the reversible NO binding in the form of a heme- $\text{Fe}^{2+}(\text{N}(\text{O})\text{SR})$ motif as an important biological strategy of NO storage.”

10. Small clusters of transition metals on TiO_2 .
Abstract of ”From single Cu atoms to sub-nanometric copper clusters deposited on TiO_2 : a DFT study”, Rutkowska-Zbik et al. [2024]:
”The growing interest in a material composed of Cu single atoms and/or their sub-nanometric clusters deposited on titania prompted us to perform systematic theoretical studies on the system comprising the anatase phase of titania, modelled by a $(\text{TiO}_2)_{34}$ cluster with copper particles of 1–7 atoms on top of it. The ground-state geometric structures were proposed and compared with the available literature data derived from EXAFS experiments done for Cu- TiO_2 materials. Copper atoms prefer to aggregate and form larger clusters on TiO_2 , as seen from the computed nucleation energies. The models were characterised by the following electronic properties: electronic band structure, natural population charges, and frontier orbitals (HOMO, LUMO, and SOMO). The copper phase becomes oxidised once it is deposited on titania. The charge distribution in the resulting structures indicates that the atoms that are the closest to the Cu- TiO_2 interface would become the active sites for catalytic processes; copper atoms would act as electrophilic, while oxygen atoms would act as nucleophilic. The calculated binding energies between the two phases show that the formation of the composite system is favourable from the thermodynamic point of view, and the interaction between the small copper clusters and the titania surface is mostly of electrostatic nature.”
11. Modeling of structure and stability of ceria-based systems as well as reactions on them. (Koleva et al. [2020, 2023], Mihaylov et al. [2021], Khivantsev et al. [2023])
Abstract of ”Comparison of the Reactivity of Platinum Cations and Clusters Supported on Ceria or Alumina in Carbon Monoxide Oxidation”, Koleva et al. [2023]:
”The mechanism of CO oxidation on platinum species supported on ceria or alumina was studied via periodic density functional calculations. In order to elucidate the nature of the catalytically active species, various reaction paths involving monoatomic species in different oxidation states- Pt^0 , Pt^{2+} , and Pt^{4+} -as well as platinum clusters were modelled. Since the oxygen centers that participate in the oxidation process may have diverse origins, the interaction of CO with the oxygen from the ceria support, dissociated O_2 molecules on the platinum species, and the oxygen molecule healing the surface oxygen vacancy in the support was considered. Ceria was modeled both as a (111) surface and as a nanoparticle, and γ -alumina was modeled as a (001) surface. The reaction paths via complexes of Pt^{2+} and Pt^{4+} cations were found to have the lowest activation barriers, 22–35 kJ/mol. The calculated activation energies on platinum clusters with high CO coverage supported on the ceria surface and the nanoparticle are also low, 40 and 19 kJ/mol, respectively. The barriers are significantly higher, 90–120 kJ/mol, when the reaction occurs on platinum supported on γ -alumina or when an oxygen preadsorbed on the platinum cluster is involved in the process. The calculations allowed us to discriminate the role of the oxidant in the modeled reaction paths and to conclude that the activation barriers are low when the oxidants are platinum species and notably higher when the oxidants are Ce^{4+} cations.”
12. Catalytic reactions in zeolites, Surface reactions, Metal oxides. (Engedahl et al. [2021, 2024], Fant et al. [2021], Levin et al. [2022], Huš et al. [2023], Sauer et al. [2024], Zhang et al. [2022], Tiburski et al. [2021], Valter et al. [2021], Lind et al. [2020], Brorsson et al. [2024, 2023], Staničić et al. [2022])
Abstract of ”Steps and catalytic reactions: CO oxidation with preadsorbed O on Rh(553)”,

Zhang et al. [2022]:

”Industrial catalysts are often comprised of nanoparticles supported on high-surface-area oxides, in order to maximise the catalytically active surface area and thereby utilise the active material better. These nanoparticles expose steps and corners that, due to low coordination to neighboring atoms, are more reactive and, as a consequence, are often assumed to have higher catalytic activity. We have investigated the reaction between CO and preadsorbed O on a stepped Rh(553) surface, and show that CO oxidation indeed occurs faster than on the flat Rh(111) surface at the same temperature. However, we do find that this is not a result of reactions at the step sites but rather at the terrace sites close to the steps, due to in-plane relaxation enabled by the step. This insight can provide ways to optimize the shape of the nanoparticles to further improve the activity of certain reactions.”

13. Surface catalysis and charge transport across materials, especially on transition metal oxides. (Snir et al. [2019], Lakhanlal and Caspary Toroker [2023], Elbaz et al. [2019], Bhargava et al. [2020])

Abstract of ”Filling the gaps on the relation between electronic conductivity and catalysis of electrocatalysts for water splitting using computational modelling”, Lakhanlal and Caspary Toroker [2023]:

”The electronic conductivity of the electrocatalyst for electrochemical water splitting reaction is critical as it involves the necessary step of charge carrier transport through the electrocatalyst. In this perspective, we have highlighted the importance of the electronic conductivity of electrocatalysts for the water splitting reaction based on recent experimental and theoretical evidence. The electronic conductivity is a crucial electronic property that directly impacts charge transport and plays a vital role in ensuring the practical effectiveness of electrocatalysts for real-world applications. We have also discussed how direct measurement (*ex-situ*) of electronic conductivity of the bulk electrocatalysts does not remain relevant when the catalyst gets restructured in actual electrolysis condition and can even change into a new phase (*in-situ*). Here, we have given our reasoned opinion about the need to model surface structures during charge transport calculations and the possibility of using several theories as well as the well-established non-equilibrium Green function (NEGF) formalism coupled with DFT for calculating the electronic conductivity of the electrocatalysts. We have discussed some recent relevant publications in which NEGF formalism has been used for current-voltage (*I-V*) calculation.”

14. Modelling crystallization, using Cellular Automata/Monte Carlo and ODE-systems to model pattern formation and vicinal growth instabilities. (Kleshtanova et al. [2023], Ivanov et al. [2023], Zaluska-Kotur et al. [2021], Popova et al. [2020])

Abstract of ”Modelling crystallization: When the normal growth velocity depends on the supersaturation”, Ivanov et al. [2023]:

”The crystallization proceeds by the advance of the crystal faces into the disordered phase at the expense of the material excess, the supersaturation. Using a conservation constraint for the transformation ratio $\alpha \in [0,1]$ as complementing the rescaled supersaturation to 1 and a kinetic law for the normal growth velocity as function of the supersaturation raised to power g , the growth order, we derive an equation for the rate of transformation $d\alpha/dt$. We integrate it for the six combinations of the three spatial dimensions $D = 1, 2, 3$ and the two canonical values of $g = 1, 2$ towards obtaining expressions for α_{Dg} . The same equation, with $g = 1$ and $D = n$ (n is the so called Avrami exponent) is obtained when taking only the linear in α term from the Taylor’s expansion around $\alpha = 0$ of the model equation of Johnson-Mehl-Avrami-Kolmogorov (JMAK). We verify our model by fitting datasets of α_{21} and α_{31} (from $\alpha = 0$ to $\alpha_{upper} = 0.999$) with JMAK to obtain from the fit $n = 1.725, 2.43$, resp. We show further how the values of n depend on the value of α_{upper} to which the fit is performed starting always from 0. Towards building a validation protocol, we start with validating α_{21} with published results.”

15. Modeling microstructure/property relations in organic bulk heterojunction for photovoltaics and

for nanocrystals for photogenerated charge extraction. (Clarke and Buxton [2024], Buxton and Clarke [2006a,b])

Abstract of "Modeling photo-generated charge extraction in bulk heterojunction nanoparticles", Clarke and Buxton [2024]:

"We present a drift-diffusion model for predicting currents generated through the absorption of solar energy inside bulk heterojunction organic nanoparticles, which are, for example, promising nanomaterials for photo-catalytic water splitting. By coupling a model of the internal microstructure of the nanoparticle with the electronic properties, we show how different characteristics of the microstructure influence the efficiency of the conversion of solar energy into electrical energy. Our model provides a foundation for using computational modeling to optimize the design of photocatalytic nanoparticles."

16. Large scale tight-binding and momentum-space Hamiltonians for moire superstructures.

Abstract of "Coupled phonons in twisted bilayer graphene", Giroto et al. [2023]

"Stacking two layers of two-dimensional materials slightly twisted relative to each other causes significant alternations of the physical properties of the resulting bilayer. For graphene, at the right twist angle, the electronic band structure features a flat band at the Fermi level that gives rise to interesting many-body physics such as correlated insulators or superconducting states. Likewise, a finite twist angle modifies the phonon band structure. A reciprocal space continuum model including lattice reconstruction due to relaxation allows us to investigate the continuous evolution of the phonon band structure with twist angle. At intermediate angles, we find a complicated structure of the phonon density of states around the frequency of the layer breathing mode, that is substantially broadened by the moiré-induced interaction with the acoustic phonon branches. We infer optical activities and suggest Raman experiments to validate our predictions. Our results suggest that suitably twisting structures may manipulate both phonon and electron properties of such a system, and thus set the stage to test electron-phonon contributions to the observed correlated states."

17. Forcefield parametrization for reactive systems. (Gutierrez-Sevillano et al. [2021], Włodarczyk et al. [2021])

Abstract of "On the design of models for an accurate description of the water – hematite interface", Gutierrez-Sevillano et al. [2021]:

"In this work we use classical methods to develop an accurate model able to describe the interactions between the molecule of water and the hematite surface. We study the variation of the interaction energy between the water molecule and the surface regarding some geometrical aspects such as the proximity to different parts of the surface, the molecule-surface distance, and the orientation of the molecule. We obtain energy profiles and compare them with results obtained using DFT. In the study we use polarizable and non-polarizable models to find out the best balance between simple and fast models, and accurate results. We found that our developed point charges model reproduces the DFT results better than a core shell model. The obtained force field parameters will make it possible to accelerate the research on the iron oxides and water interfaces used in the description of the water-splitting reaction, which is a low-emission hydrogen source."

18. Transport properties of graphene and MoS₂. (Vancsó et al. [2013], Márk et al. [2017])

Abstract of "Electronic transport through ordered and disordered graphene grain boundaries", Vancsó et al. [2013]:

"The evolution of electronic wave packets (WPs) through grain boundaries (GBs) of various structures in graphene was investigated by the numerical solution of the time-dependent Schrödinger equation. WPs were injected from a simulated STM tip placed above one of the grains. Electronic structure of the GBs was calculated by ab-initio and tight-binding methods. Two main factors governing the energy dependence of the transport have been identified: the misorientation angle of the two adjacent graphene grains and the atomic structure of the GB."

In case of an ordered GB made of a periodic repetition of pentagon-heptagon pairs, it was found that the transport at high and low energies is mainly determined by the misorientation angle, but the transport around the Fermi energy is correlated with the electronic structure of the GB. A particular line defect with zero misorientation angle Lahiri et al., behaves as a metallic nanowire and shows electron-hole asymmetry for hot electrons or holes. To generate disordered GBs, found experimentally in CVD graphene samples, a Monte-Carlo-like procedure has been developed. Results show a reduced transport for the disordered GBs, primarily attributed to electronic localized states caused by C atoms with only two covalent bonds.”

19. Electronic and optical properties of defects in 2D materials. (Vancsó et al. [2016, 2019b], Dobrik et al. [2021])

Abstract of ”Large-area nanoengineering of graphene corrugations for visible-frequency graphene plasmons”, Dobrik et al. [2021]:

”Quantum confinement of the charge carriers of graphene is an effective way to engineer its properties. This is commonly realized through physical edges that are associated with the deterioration of mobility and strong suppression of plasmon resonances. Here, we demonstrate a simple, large-area, edge-free nanostructuring technique, based on amplifying random nanoscale structural corrugations to a level where they efficiently confine charge carriers, without inducing significant inter-valley scattering. This soft confinement allows the low-loss lateral ultra-confinement of graphene plasmons, scaling up their resonance frequency from the native terahertz to the commercially relevant visible range. Visible graphene plasmons localized into nanocorrugations mediate much stronger light–matter interactions (Raman enhancement) than previously achieved with graphene, enabling the detection of specific molecules from femtomolar solutions or ambient air. Moreover, nanocorrugated graphene sheets also support propagating visible plasmon modes, as revealed by scanning near-field optical microscopy observation of their interference patterns.”

20. Magnetic properties of nanoribbons and defects. (Magda et al. [2014], Vancsó et al. [2019a], Koós et al. [2019])

Abstract of ”Room-temperature magnetic order on zigzag edges of narrow graphene nanoribbons”, Magda et al. [2014]:

”The possibility that non-magnetic materials such as carbon could exhibit a novel type of s–p electron magnetism has attracted much attention over the years, not least because such magnetic order is predicted to be stable at high temperatures. It has been demonstrated that atomic-scale structural defects of graphene can host unpaired spins, but it remains unclear under what conditions long-range magnetic order can emerge from such defect-bound magnetic moments. Here we propose that, in contrast to random defect distributions, atomic-scale engineering of graphene edges with specific crystallographic orientation—comprising edge atoms from only one sub-lattice of the bipartite graphene lattice—can give rise to a robust magnetic order. We use a nanofabrication technique⁴ based on scanning tunnelling microscopy to define graphene nanoribbons with nanometre precision and well-defined crystallographic edge orientations. Although so-called ‘armchair’ ribbons display quantum confinement gaps, ribbons with the ‘zigzag’ edge structure that are narrower than 7 nanometres exhibit an electronic bandgap of about 0.2–0.3 electronvolts, which can be identified as a signature of interaction-induced spin ordering along their edges. Moreover, upon increasing the ribbon width, a semiconductor-to-metal transition is revealed, indicating the switching of the magnetic coupling between opposite ribbon edges from the antiferromagnetic to the ferromagnetic configuration. We found that the magnetic order on graphene edges of controlled zigzag orientation can be stable even at room temperature, raising hopes of graphene-based spintronic devices operating under ambient conditions.”

4 Theoretical methods, ranges and limitations

It is quite important to be aware what the range and applicability of any given method is. Here we asked our participants to detail what they use and their assessment regarding its strengths and weaknesses. Since there is a lot of overlap in the methods, we summarize the results:

Density functional theory (DFT) is the method of choice for electronic structure and ground state calculations. Nine (9) out of fifteen (15) participants explicitly mention its use in one form or another, which include its variations such as constrained DFT (Kaduk et al. [2011]), TD-DFT and hybrid DFT (use case Platonenko et al. [2024]). Additional uses are UV-Vis spectra, embedding and combination of DFT with MD (Ab Initio Molecular Dynamics). Other provided references are (Cohen et al. [2008], Liang et al. [2021a], Zhang and Bieberle-Hütter [2016], George et al. [2019a, 2020], Zhang et al. [2016]).

Regarding the limitations of DFT, José R. B. Gomes comments that the unit cells for the DFT calculation are rather small and the influence of the solvent is neglected in almost 100% of the cases.

Embedding methods: Combine different levels of theory in one computation, for example quantum chemistry embedded in DFT. (Libisch et al. [2014])

Tight binding: Large-scale Hamiltonians (millions of atoms), but effective single-particle theory. Proper parameterization is necessary, for instance employing machine learning. (Schattauer et al. [2022]) Once obtained, a tight-binding hamiltonian may be used for many-body calculations with methods requiring a reduced-complexity effective Hamiltonian or for transport and LDOS calculations, see Fig. 1.

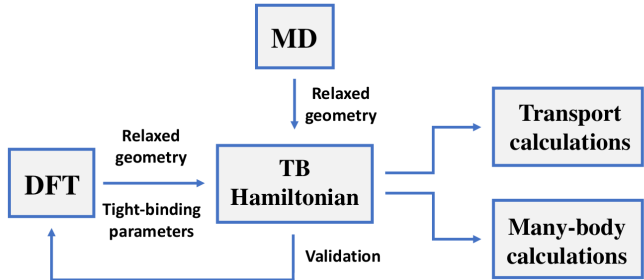


Figure 1: Sketch of the multiscale numerical simulation scheme used by Péter Vancsó to obtain tight binding parameters.

Hubbard-model for magnetic calculations - for large systems mean-field approximation is necessary. (Péter Vancsó)

Wave packet dynamical (WPD) transport simulations - large systems can be investigated above 100.000 atoms; potential is required. (Péter Vancsó)

Use cases employing phenomenological models are a large range of materials, including oxides, metals, sulfides, carbides, and zinc-blende semiconductors. (Reichman and Caspary Toroker [2023], Snir et al. [2019]) (Maytal Caspary Toroker)

Drift - diffusion models for excitonic organics, suitable for modelling exciton generation, electron/hole dissociation and transport in heterogeneous materials. Suitable for transport over length

scales ranging from nanometers to hundreds of nanometers. Molecular specific physics, such as excited state energy levels and charge hopping rates, are used as inputs for the models. (Clarke and Buxton [2024], Buxton and Clarke [2006a,b])

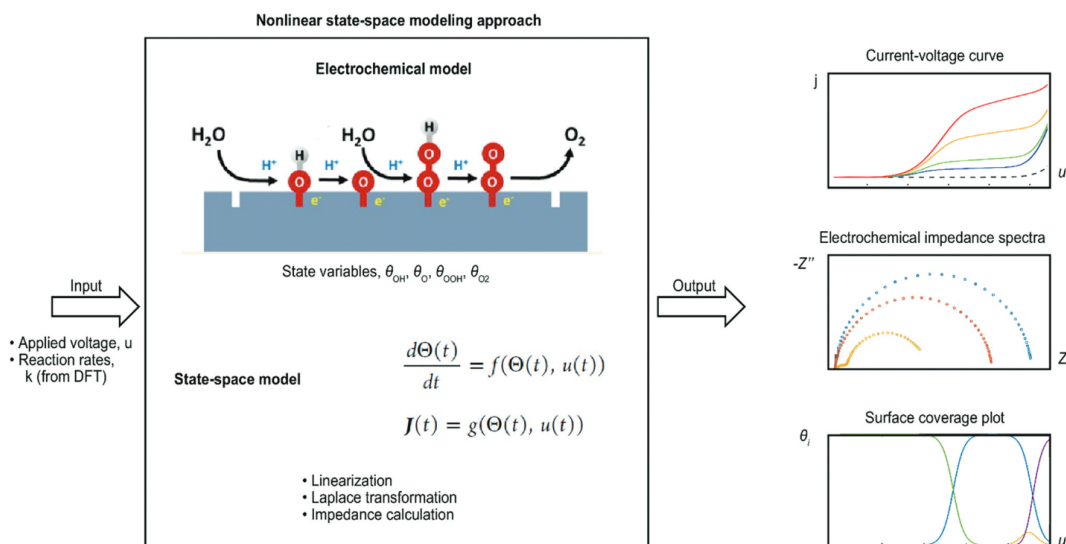


Figure 2: Sketch of Nonlinear State-space Approach approach for simulating electrochemical data of the oxygen evolution reaction provided by Anja Bieberle-Hütter (figure 4 in Samanta et al. [2022])

Kinetic Monte Carlo (KMC) models for excitonic organics, suitable for modelling exciton generation, electron/hole dissociation and transport in heterogeneous materials. These models are similar in scope to drift-diffusion methods, but charge hopping is explicitly modelled. KMC methods not used for water splitting nanocrystals. (Jones et al. [2014], Lyons et al. [2012, 2011])

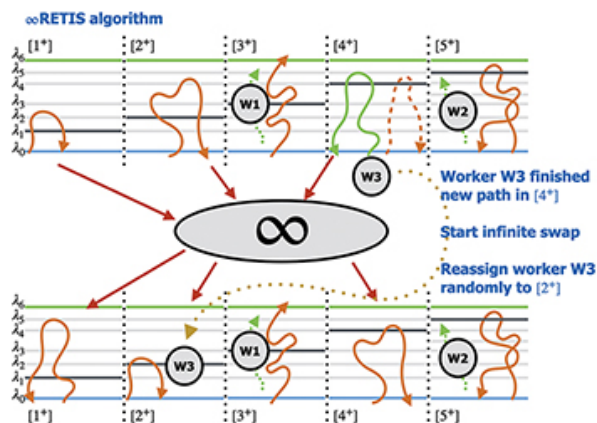


Figure 3: Sketch of InfinityRETIS by Titus van Erp.

Replica exchange transition interface sampling (RETIS) was employed (van Erp [2007]), see Fig. 3, which is an improvement to the transition interface sampling TIS (transition interface

sampling) method (van Erp et al. [2003]). In the earlier mention ref (Zhang et al. [2024]), RETIS was further improved to be highly scalable. (The approach was called InfinityRETIS.)

Strong points: It is an exact method, which means it will provide the same rate, reaction mechanism as brute force MD, but exponentially faster **Weak points:** It works for fast rare events. If it happens, it should happen fast. If the transition event duration is slow, approximate methods are needed such as the REPPTIS method. (Vervust et al. [2023]) (Titus van Erp)

Péter Vancsó elaborates: The microscopic mechanical and electronic modelling are based on molecular dynamics and density functional theory calculations. After adopting reliable fitting parameters, the tight-binding Hamiltonian can be constructed for the electronic structure calculations. The well parametrized TB Hamiltonian also serve as a simple starting point for the transport calculations and the inclusion of many-body effects.

The remaining listed methods are

1. Microkinetic modelling (van den Boorn et al. [2022])
2. Molecular dynamics
3. Transfer matrix method, solving ODE-systems, scaling analysis, Cellular Automata (Vesselin Tonchev)
4. Data Mining, AI (Anders Hellman)
5. DDEC6 charges and bonding indices, NCI (Non-Covalent Interaction Index), Force-Matching method for ReaxFF Force Fields parametrization (Bartek Szyja)

5 Codes

We asked the participants which codes they use, if these are commercially available or custom made, and provide points of contact if possible.

Many listings are commercially available packages with a wide range of available methods. For instance, molecular dynamics calculations can be both done via LAMMPS and VASP; the latter also happens to be most used DFT code. In the following we associate the method with the codes listed by the participants. We do not imply that these codes are only used for this specific method, but rather reproduce the answers of the participants.

1. For electronic structure and in particular **Density Functional Theory** the used codes are VASP, GPAW, SIESTA, CP2K, TURBOMOLE, CRYSTAL, MOLPRO and GAUSSIAN.
2. For **Molecular Dynamics** GROMACS and LAMMPS are also mentioned.
3. Chargemol is used for **DDEC6 charges** and **bonding indices**. (Bartek Szyja)
4. For **Force Fields** we have GULP. Forcematching is done by Bartek Szyja inhouse.
5. **Molecular Orbit Analysis:** Aomix
6. **Catalysis Kinetics Calculations:** PyCatKin (Anders Hellman)

The remaining software in use are custom made.

1. **Tight Binding** (Florian Libisch, Péter Vancsó) (Libisch et al. [2014], Schattauer et al. [2022])

2. **Embedding** formalism available from E. A. Carter.
3. **Rare event molecular simulations**: pyretis (Lervik et al. [2017], Riccardi et al. [2019], Vervust et al. [2024]) and InfinityRETIS (Titus van Erp)
4. **Monte Carlo**: RASPA (Sofia Calero)
5. **Visualization**: iRASPA (Sofia Calero)
6. **Microkinetic Modelling** (Anja Bieberle-Hütter)
7. **Hubbard-model** (Péter Vancsó)
8. **Wave Packet Dynamic Transport Simulations** (Péter Vancsó)
9. **ODE solving** (Vesselin Tonchev)
10. **Kinetic Monte Carlo** (Nigel Clarke)
11. **Drift-Diffusion** (Nigel Clarke)

Finally, Maytal Caspary Toroker lists the recordings on a Material Training School (Neufeld and Toroker [2016])

6 Accuracy and Scaling of Methods

Lastly, we ask the participants about the accuracy and scaling of their methods of choice. These are their answers, with the method added in parentheses where necessary for clarity.

Anja Bieberle-Hütter: Our accuracy is determined by the input values that we need. Examples of our challenges:

- 1) Rate constants we estimate through **DFT** - hence, accuracy of DFT, but this is actually not the problem, but more the fact that DFT is at a gas-solid interface and 0 K, but our real system that we are modeling is a liquid-solid interface and at room temperature.
- 2) A lot of input values that we need for our modeling are not known, think of electron, hole, trap state densities for a specific system under specific operation, material specific parameters. (**microkinetic modeling**)

Sofia Calero: Our methods are very accurate in porous, crystalline systems if we have force fields available. With this method scalability is not possible. (**Monte Carlo**)

Maytal Caspary Toroker: The method for charge transport calculations has been verified by material comparison and benchmarking against experiment. (**Wave packet propagation, surface heterogeneous catalysis, phenomenological models**)

Nigel Clarke: The accuracy of our methods is dependent on the accuracy of the parameterisation. This is an area of research requiring development, since many parameters are difficult to measure experimentally. Building multiscale models that incorporate both DFT for electronic structure and Molecular Dynamics for transport would greatly enhance our methods, allowing them to be applied to specific chemistries. (Drift Diffusion models, Kinetic Monte Carlo)

José R. B. Gomes: (**Computational Chemistry, DFT, Force-Fields**) Accuracy is usually determined by the realistic nature of the model (often it is oversimplified in order to allow the calculations to run in a short time). Most methods scale pretty well and the problem is related to the lack of sufficient computational resources.

Florian Libisch: **Tight-binding**: needs to be parametrized Schattauer et al. [2022], but can treat millions of atoms. We can calculate transport, LDOS, optical properties, or derive effective Hamiltonians of reduced dimensionality that are then used for some correlated techniques. **Embedding** allows for combining different levels of theory in one calculation, for example correlated-wavefunction approaches in DFT Libisch et al. [2014], Schäfer et al. [2021], or for hybrid functionals in conventional DFT Libisch et al. [2017].

Anders Hellman: The **DFT** part is standard. The **microkinetic modeling** and the **kinetic Monte-Carlo** is system dependent (timescale 1s).

Eugene Kotomin: best available for large scale materials modelling (**hybrid DFT**)

Dorota Rutkowska-Żbik: The accuracy is typical of **DFT**; for the bigger systems I search the conformational space with **MM** methods.

Bartek Szyja: The main limitation is the treatment of the electronic structure from **DFT**. It affects both - **CDFT** method, where it is used self-consistently with respect to the constraint, and **ReaxFF** parameter fitting, where it is used as a reference.

Sergei Piskunov: High accuracy up to 200-300 atoms. (**Density Functional Theory, excited states UV-Vis spectra**)

Vesselin Tonchev: **Transfer Matrix** method uses an one-step coarse graining.

Titus van Erp: InfinityRETIS is exact, which means you obtain identical results as the brute force MD simulation, but exponentially faster. The InfinityRETIS method is highly scalable as it uses asynchronous replica exchange MC moves with infinite swapping. It allows you to run it on a number of nodes in parallel. (**replica exchange transition interface sampling**)

Péter Vancsó: In my methods accurate DFT calculations on small systems serve as an input for the other methods. For example large scale WPD (**Wave packet dynamical**) calculations are based on proper potentials fitted to the DFT band structure results. These band structures are also the input for my TB (**Tight-Binding**) and **Hubbard** calculations.

7 Participants

Finally, we provide a compact listing of all the participants, their occupations, affiliated institutes and e-mail addresses.

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Glossary

Cellular Automata Cellular Automata are discrete, abstract computational systems that have found extensive applications in modeling complex systems with simple rules applied on a grid-like architecture.

They are used to model a wide range of phenomena including biological and chemical processes, spread of diseases, traffic flow, and urban development.

. 4

Defect modeling Defect Modeling involves the simulation and analysis of imperfections in the atomic or molecular structure of materials, such as vacancies, interstitials, and dislocations.

This modeling is critical in understanding material properties such as strength, electronic and thermal properties, which are influenced by the presence of defects.

. 3

Drift Diffusion models Drift Diffusion Models are used to describe the transport of particles, typically electrons and holes, under the influence of an electric field and thermal diffusion.

These models are crucial in the design and analysis of semiconductor devices, solar cells, and integrated circuits where charge transport is key.

. 15

Electrocatalysis Electrocatalysis involves chemical reactions that are facilitated at the surface of electrodes with the help of an applied electric potential. The combination of applied potential and catalyst alters the rate by either increasing or decreasing it, thanks to the presence of the catalyst.

Widely applied in fuel cells, electrolyzers for hydrogen production, and batteries, electrocatalysis is crucial for energy conversion and storage solutions.

. 2

Embedding methods Embedding Methods are computational techniques where a highly accurate treatment of a small part of the system (often where chemical reactions occur) is embedded within a larger system that is treated at a lower level of theory.

These methods are used in quantum chemistry to study reactions in complex environments, such as enzyme reactions in biochemical systems or catalytic processes in inhomogeneous catalysts.

. 3

Kinetic Monte Carlo Kinetic Monte Carlo methods are a set of algorithmic approaches used to simulate the time evolution of processes that occur in systems out of thermodynamic equilibrium.

Used in surface science to model surface reactions, adsorption processes, and in materials science for diffusion of impurities and phase transformations.

. 15

Micro-kinetic models Micro-kinetic modeling involves the use of detailed reaction mechanisms to predict the behavior and rate of catalytic reactions. These models consider all the elementary reaction steps and their kinetics to provide insights into the dynamics of the catalytic process.

They are crucial for designing catalysts and optimizing reaction conditions in industrial processes. Micro-kinetic models help in understanding how changes in operating conditions affect the performance of catalysts and aid in the scale-up of catalytic reactions.

. 3

Molecular Dynamics (MD) Molecular Dynamics is a computer simulation method used to study the physical movements of atoms and molecules. The atoms and molecules are allowed to interact via, e.g., **ReaxFF force-fields** for a period of time, providing the means for a dynamic evolution of the system.

MD is extensively used in material science, biophysics, and chemistry to study the structure, dynamics, and thermodynamics of biological macromolecules and material responses under different conditions

. 3, 4

Monte Carlo techniques Monte Carlo techniques are a broad class of computational algorithms that rely on repeated random sampling to obtain numerical results. These methods use probability and statistical mechanics to predict and analyze complex systems.

In the context of catalysis, Monte Carlo methods are used to simulate adsorption isotherms, diffusion of molecules on catalyst surfaces, and to model reaction networks under uncertain conditions.

. 3

Photocatalysis Photocatalysis refers to the acceleration of a photoreaction in the presence of a catalyst. In photocatalytic processes, the catalyst is activated by the absorption of light, typically UV or visible light, to create electron-hole pairs that can then promote chemical reactions. Photocatalysis is used to directly harness solar energy for environmental remediation (e.g., degradation of pollutants in water and air) and energy conversion technologies, such as water splitting to generate hydrogen.. 2

ReaxFF Force Fields ReaxFF is a reactive force field designed to model chemical reactions with atomistic potentials without needing predefined reaction pathways, allowing the simulation of reactions dynamically.

It is used in MD simulations that require the formation or breaking of chemical bonds, such as combustion, catalysis, and material degradation processes.

. 14

State-space Approach The state-space approach is a mathematical framework used for modeling and analyzing systems that are described by a set of inputs, outputs, and state variables. This model represents the system as a set of first-order differential (or difference) equations, capturing the dynamics of the system in terms of its state variables, which evolve over time based on these equations. The state-space model is versatile and can represent linear, non-linear, time-variant, and time-invariant systems.

In engineering, the state-space approach is widely used for control system design, including aerospace vehicles, automotive engineering, and robotics. It enables the implementation of modern control techniques, such as optimal control and state feedback control. In economics, it helps in estimating dynamic economic models. It is also applied in signal processing for designing and analyzing filters and in electrical engineering for circuit analysis.

. 13

Tight Binding Tight binding is a semi-empirical method to calculate the electronic band structure using a simple model of the potential seen by the electrons in a solid. It typically focuses on the interaction between nearest neighbors and assumes that atomic orbitals overlap slightly.

Tight binding is applied in solid state physics to predict electronic properties of materials, aiding in the development of semiconductors and nanotechnology devices.

. 14

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