



Deep Materials:
Perspectives on data-driven materials research

Monday 10th 2018 – Friday 14th 2018

Dresden | Germany

BOOK OF ABSTRACTS

This summer school is part of TU Dresden's Institutional Strategy, funded by the Excellence Initiative of the German Federal and State Governments. The school receives additional funding through the Helmholtz Excellence Network DCM-MatDNA.

PROGRAM

	10-Sep-18	11-Sep-18	12-Sep-18	13-Sep-18	14-Sep-18
	Monday	Tuesday	Wednesday	Thursday	Friday
09:00-09:30	opening	Cecilia Clementi (Rice)	Jörg Behler (U Göttingen)	M. Mosch (SLUB) J. Vieten (DLR Köln)	N. Marzari (EPFL)
09:30-10:00	Roger French (Case Western)				
10:00-10:30					
10:30-11:00					
11:00-11:30	coffee break	coffee break	coffee break	coffee break	R. French (Case Western)
11:30-12:00	Thomas Lehmann (TU Dresden)	Pasquale Pavone (HU Berlin)	K. Thygesen (DTU) D. Urban (Fraunhofer IWM) P. Steinbach (Scionics)	luncheon	
12:00-12:30					
12:30-13:00					
13:00-13:30	luncheon	luncheon	luncheon	luncheon	Round Table with Participants
13:30-14:00					
14:00-14:30	Dominik Alfke (TU Chemnitz)	Frank Noe (FU Berlin)	Kristian Sommer Thygesen (DTU)	J. Schuster (ENAS Chemnitz) R. Scholz (IAPP, Dresden) M. Vaez Allaei (Uni. Tehran)	
14:30-15:00					
15:00-15:30					
15:30-16:00	coffee break	coffee break	coffee break	coffee break	
16:00-16:30	hands on	hands on	hands on	contributed talks	
16:30-17:00					
17:00-17:30	Get-to-Know	Poster Session			
17:30-18:00					
18:00-19:00					
19:00-20:00					
20:00-20:30					

Lectures

Dominik Alfke	Introduction to Graph-based Learning
Jörg Behler	High Dimensional Neural Network Potentials
Cecilia Clementi	Learning effective molecular models from experimental observables
Connor Coley	Machine Learning for Synthetic Chemistry
Roger French	Computer Vision and Machine Learning in a Distributed Computing Environment: Photovoltaic Degradation Quantified Using Electroluminescent Images
Thomas Lehmann	Introduction to Machine Learning with Python
Frank Noe	Machine Learning for Molecular Dynamics
Pasquale Pavone	Concepts, Challenges, and Results of the NOMAD (Novel Materials Discovery) Laboratory
Kristian Sommer Thygesen	Building a computational materials database

Invited Speakers

Roger French	Time Series Analysis and Network Modeling of PV Modules and Power Plants to Decrease Degradation Rates
Nicola Marzari	Computational design and discovery of novel materials
Marc Mosch	The Material HUB
Reinhard Scholz	Thermally activated delayed fluorescence - A new route to more efficient OLEDs?
Jörg Schuster	Simulation of Materials, Processes and Devices for Nanoelectronics Engineering
Kristian Sommer Thygesen	High-throughput discovery of new light absorbing semiconductors
Peter Steinbach	Where no CPU has gone before: GPUs for Deep Learning
Daniel Urban	A machine-learning approach for the discovery of novel hard-magnetic phases
S. Mehdi Vaez Allaei	Phononic heat transport and thermal rectification in low dimensional heterostructures
Josua Vieten	Perovskite Materials design for two-step thermochemical processes

Contributed Talks

Tuan Nguyen	Design of bio-inspired materials: Emerging innovation from deep learning
Nikita Sengar	Bayesian Optimization to Model Polymorphism and Phase Transition Mechanisms in Small Molecule Organic Semiconductors
Antonis-Charalampos Stellas	Smart nanometrology with Machine Learning

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LECTURES

DOMINIK ALFKE

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Graph based methods for data science

The purpose of this talk is to give an introduction to tools and methods for data science applications when the data has the structure of a graph or hypergraph. We discuss how to build graphs from general data sets and encode their behaviour in the graph Laplacian operator. We present increasingly sophisticated approaches from Spectral Clustering to Graph Convolutional Neural Networks as well as possible applications.

Biography

Dominik Alfke studied mathematics at the Otto-von-Guericke-University and focused on Optimization, Finite Element Methods and Model Order Reduction. Since October 2017, he is a PhD student at the Chair of Scientific Computing at Technische Universität Chemnitz.



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JÖRG BEHLER

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High Dimensional Neural Network Potentials

A lot of progress has been made in recent years in the development of atomistic potentials employing machine learning (ML) techniques. In contrast to most conventional potentials, which are based on physical approximations and simplifications to derive an analytic functional relation between the atomic configuration and the potential-energy, ML potentials rely on simple but very flexible mathematical terms without a direct physical meaning. Instead, in case of ML potentials the topology of the potential-energy surface is “learned” by adjusting a number of parameters with the aim to reproduce a set of reference electronic structure data as accurately as possible. Due to this bias-free construction they are applicable to a wide range of systems without changes in their functional form, and a very high accuracy close to the underlying first-principles data can be obtained. Neural network potentials (NNPs), which have first been proposed about two decades ago, are an important class of ML potentials. While the first NNPs have been restricted to small molecules with only a few degrees of freedom, they are now applicable to high-dimensional systems containing thousands of atoms, which enables addressing a variety of problems in chemistry, physics and materials science. In this lecture the basic ideas of NNPs are presented with a special focus on constructing NNPs for high-dimensional condensed systems. A recipe for the construction of these potentials is given and remaining limitations of the method are discussed.

Biography

Prof. Dr. Behler studied Chemistry at the University of Dortmund from 1995 to 2000 and did his PhD at the Fritz-Haber-Institute der Max-Planck-Gesellschaft in Berlin. After several Postdoc employments he became a Independent Junior Research Group Leader in the topic of Theoretical Chemistry at Ruhr-Universität Bochum for the period 2008 to 2017. Since 2017 he is a Full Professor for Theoretical Chemistry (W3) at the Universität Göttingen.

His main research fields refer to the development of machine learning potentials for applications in materials science as well as chemical processes at interfaces and chemistry in aqueous solutions.



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CECILIA CLEMENTI

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Learning effective molecular models from experimental observables

Recent breakthroughs in experimental technologies and in high-performance computing have enabled unprecedented measurements and simulations of complex systems such as macromolecules. However, experiments provide only a partial view of macromolecular processes and are limited in their temporal and spatial resolution. On the other hand, atomistic simulations are still not able to sample the conformation space of large complexes, thus leaving significant gaps in our ability to study molecular processes at a biologically relevant scale. We present recent efforts to bridge these gaps, by using experimental data as a starting point in a computational modelling approach. Models at different resolutions can be “anchored” to experimental measurements, to provide quantitatively accurate representations of systems of interest, and address open physical questions.

Biography

Dr. Cecilia Clementi received her B.S. in Physics from the University of Florence, Italy and her M.Sc. and PhD in Physics from the International School for Advanced Studies (SISSA/ISAS) in Trieste, Italy. She was a La Jolla Interfaces in Science postdoctoral fellow at University of California San Diego before joining the faculty in the Department of Chemistry at Rice University, in Houston, Texas USA in 2001. She is currently also a Senior Investigator in the Center for Theoretical Biological Physics (CTBP) at Rice, and an Einstein Visiting Professor at the Freie Universität in Berlin, Germany.

Dr. Clementi's research focuses on the modeling of biomolecular dynamics over a broad range of time and length scales.



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CONNOR COLEY

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Machine Learning for Synthetic Chemistry

The identification and synthesis of small molecules that exhibit a desired function is an essential part of challenges in the development of specialty polymers, organic photovoltaics, and medicines. The typical discovery paradigm is an iterative process of designing candidate compounds, synthesizing those compounds, and testing their performance, where each repeat of this cycle requires weeks or months. Time and cost constraints may necessitate selecting compounds on the basis of what are perceived as fast to synthesize, rather than what are most informative to assay.

This talk will cover our recent progress in the application of data science and machine learning techniques to problems in synthetic chemistry as they relate to the discovery process. I will describe how historical reaction data can be used to inform decision-making in small molecule pathway design, for both retrosynthesis and forward reaction prediction. I will also summarize some techniques in molecular property prediction and an approach to de novo molecular design using a neural model capable of graph generation. The overall aim of our work is to systematize and streamline the process by which new functional small molecules are designed and synthesized.

Biography

Connor W. Coley received his B.S. in Chemical Engineering from Caltech and M.S. in Chemical Engineering Practice from MIT. He is a final-year Ph.D. Candidate with professors Klavs F. Jensen and William H. Green at MIT working on various aspects of computer-assistance and automation for organic synthesis, including both computational planning and experimental execution. His recent work under the DARPA Make-It program and the newly-formed Machine Learning for Pharmaceutical Discovery and Synthesis (MLPDS) Consortium focuses on the development of a data-driven synthesis planning program and in silico strategies for predicting the outcomes of organic reactions. His work in the field of machine learning and synthetic chemistry has earned him the distinction of being a DARPA Riser and one of C&EN's Talented 12.



His current work focuses on different forms of computer-assistance to chemical synthesis, including application of microfluidic platforms for the resource-efficient development and optimization of chemical processes and machine learning-driven approaches to leverage historical chemical data for designing synthetic routes.

YOUR NOTES:

[illegible]

ROGER FRENCH

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Computer Vision and Machine Learning in a Distributed Computing Environment: Photovoltaic Degradation Quantified Using Electroluminescent Images

Data Science can be applied to small or large datasets and at the SDLE Research Center our focus on Lifetime & Degradation Science (L&DS)¹ requires analysis of large time-series, spectral and image datasets. For L&DS research we use Hadoop², Hbase and Spark v2.2 to ingest, analyze and model these in our Common Research Analytics and Data Lifecycle Environment (CRADLE)² which (version 2.2) has 92 TB of disk storage, 180 cores and 2 Tb of RAM. The three major tasks of CRADLE is: 1) to store large volumes of de-identified and diverse datasets 2) to efficiently query, analyze and model these data. 3) to write back analytical results and metadata. Hbase is a NoSQL database which stores data as triples, enables sparse tables and doesn't have fixed table schema. CRADLE is embedded in the CWRU HPC cluster providing access to 4000 CPU cores and 100,000 GPU cores, we run parallel analyses using fleets of SLURM jobs. Spark provides in-place and in-memory analytics thus considerably improving the processing time. We are also planning to implement HGraphDB, a graph-database, for our structural equation and Bayesian network modeling.

Electroluminescent (EL) imaging of PV modules can provide insights to degradation mechanisms, but has only recently been quantitatively analyzed.³ We have built an automated pipeline for image processing using computer vision to extract high dimensional features which best describe these images followed by supervised and unsupervised machine learning.⁴ Supervised classification of PV cells into corroded, cracked and good (non-degraded) classes, Support Vector Machine (SVM) showed an accuracy of 98% and was 10 times faster than Convolutional Neural Networks (CNN). For unsupervised classification features are extracted from PV cell images using Gray Level Co-Occurrence Matrix (GLCM), followed by principal component analysis (PCA) on the extracted features to reduce the dimensionality.⁵ Hierarchical clustering is then applied on the principal components to cluster the images into degraded and non-degraded PV cells. The coherence of the hierarchical clusters is 78 %.

Biography

Roger H. French is the Kyocera Professor of Ceramics in the Case School of Engineering, Case Western Reserve University, Cleveland, Ohio. He has secondary appointments in Macromolecular Science, Biomedical Engineering, and Physics. He is the faculty director of the CWRU Applied Data Science program which offers a minor university-wide. He is the director of the SDLE Research Center at CWRU, an Ohio Third Frontier, Wright Project center focused on lifetime and degradation science of long lived technologies and data science and analytics. Prior to joining Case Western Reserve in 2010, French was a Research Fellow in Central Research and Development, DuPont Co. (starting in 1985) and Adjunct Professor of Materials Science, University of Pennsylvania (from 1994). He received his B. S. from Cornell University and his Ph.D. from Massachusetts Institute of Technology, both in Materials Science.



Using vacuum ultraviolet and optical spectroscopies, spectroscopic ellipsometry, and computational optics, his research is in optical properties, electronic structure, and radiation durability of optical materials, polymers, ceramics, and liquids.

YOUR NOTES:

[illegible]

THOMAS LEHMANN

Technische Universität Dresden, Germany

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Introduction to Machine Learning with Python

In a hands-on session on machine learning we discuss the application of various methods, starting from Linear Regression to Random Forests and Cluster Analysis. Apart from a theoretical discussion of those concepts, we will start to implement them in Python. Please bring your own laptop and brush up your programming skills.

Biography

Thomas Lehmann is a Theoretical Physicist with a focus on numerical modelling of quantum transport in nanostructures and molecular electronics. He studied Physics at the TU Dresden and is currently finishing his PhD thesis in the group of Prof. Cuniberti. His work is in cooperation with the International Max Planck Research School and the International Graduate School iEGSEMP: Korea with research stays at POSTECH (Korea), CEMES-CNRS (France) and UNIST (Korea). Since becoming interested in Machine Learning methods, he has been awarded a Data Science Fellowship at ASI Data Science in London. He has been working for easyJet to develop a dynamic pricing model for seat allocations by predicting the time-evolution of customer demand. He is now looking into applications of Machine Learning models for materials science.



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FRANK NOE

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Machine Learning for Molecular Dynamics

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Biography

Frank Noé studied his Bachelor of Science in Electrical Engineering in Stuttgart. He worked in an artificial intelligence start-up company in Frankfurt, and then moved to Cork, Ireland where he obtained his M.Sc. in computer science in 2002. Frank completed his Ph.D. in Biophysics with Jeremy Smith at University of Heidelberg in 2006. In 2007, he started his research group at the Matheon research center at Freie Universität Berlin, and received tenure in 2013 in the same location, where he holds an interdisciplinary chair between Mathematics, Physics and Chemistry. Frank received two awards of the European Research Council, an ERC starting grant in 2012 and a ERC consolidator grant in 2017. He is adjunct professor at the Chemistry department of Rice University since 2015.



YOUR NOTES:

[illegible]

PASQUALE PAVONE

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Concepts, Challenges, and Results of the NOMAD (Novel Materials Discovery) Laboratory

The NOMAD (Novel Materials Discovery) Laboratory Center of Excellence (CoE), <https://NOMAD-CoE.eu>, is a community-driven activity with the mission to serve the whole field of materials science and engineering. It tackles the issues of Big Data in materials science, starting from the NoMaD Repository, which by now contains results from more than 18 million DFT total-energy calculations. This corresponds to several billion CPU-core hours spent on high-performance computers worldwide. With these and more and more incoming data, we build a Materials Encyclopedia, to provide a user-friendly access to all these results, also making use of Advanced Graphics. Novel Big-Data Analytics tools are developed for finding trends, identifying outliers, and predicting new materials with tailored properties. Thus, this talk describes the basic concepts and goals of the NOMAD CoE in order to stimulate a discussion and suggestions on how to proceed further.

Biography

Pasquale Pavone did his Master of Science in Physics at the University of Messina in Italy. From 1987 to 1991, he made his PhD at the International School for Advanced Studies in Trieste and went to the University of Regensburg, joined the group of Prof. Strauch and got his postdoctoral lecture qualification in the year 2002. After that, he was a Scientific Application Specialist in Copenhagen (Denmark) and worked as a Senior Scientist and Lecturer at Materials Center Leoben & University of Leoben in Austria. Since 2011, he is working at Humboldt-Universität zu Berlin as a Senior Staff Scientist and Lecturer in the field of Coordination and development of the exciting code.



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KRISTIAN SOMMER THYGESEN

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Building a computational materials database

For more than a century, experimental databases on e.g. structural, thermal, and electronic properties, have been a cornerstone of materials science, and in the past decade, the experimental data have been augmented by an explosion of computational data obtained from first-principles calculations. Strong efforts are currently being focused on storing and organising the computational data in open repositories. Some of the larger repositories, together containing millions of DFT calculations, are the Materials Project, the Automatic Flow for Materials Discovery (AFLOWLIB), the Open Quantum Materials Database (OQMD), and the Novel Materials Discovery (NOMAD) Repository.

In this talk I will discuss our efforts to construct a computational database of two-dimensional materials. The database currently contains a large variety of properties of 2500+ materials distributed over more than 40 crystal structures. Material properties are systematically calculated by density functional theory and many-body perturbation theory following a semi-automated workflow for maximal consistency and transparency. I will present the structure of the workflow and the database and discuss what we have learned in the process of the project. Finally, I will give some examples to illustrate the use of the database for identifying trends and correlations and for discovery of novel materials.

Biography

Prof. Kristian S. Thygesen earned his PhD degree in Physics from the Technical University of Denmark (DTU) in 2005. After a post doctoral position at Freie University Berlin he returned to DTU where he became Associate Professor in 2010 and leader of the Molecular Electronics group at the Lundbeck Foundation's Center for Atomic-scale Materials Design (CAMD). He was Director of NanoDTU from 2009-2010 and has been Spokesperson for Psi-k working group on Quantum Transport in Nanostructures since 2009. In 2013 he became Professor at the Department of Physics at DTU and in 2015 he became leader of the Section for Computational Atomic-scale Materials Design.



Recently, his research focuses on the development of first-principles methods for the description of ground- and excited state properties of solids and low-dimensional systems. He co-develops the GPAW electronic structure code, and the Computational Materials Repository (<http://c2db.fysik.dtu.dk/>), holds the ERC grant LIMA, and is member of the Center for Nanostructured Graphene (<http://www.cng.dtu.dk>) and the Center for Novel Materials Discovery (<https://www.nomad-coe.eu>)

YOUR NOTES:

[illegible]

INVITED SPEAKERS

ROGER FRENCH

Case Western University, USA

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Time Series Analysis and Network Modeling of PV Modules and Power Plants to Decrease Degradation Rates

As solar power grows, it becomes critical to fully understand and predict the power output of photovoltaic (PV) modules over their entire > 30 year lifetimes. Traditional PV module degradation tests are done under lab-based accelerated exposure environments, with the intent of testing the PV lifetime within a reasonable time scale. The new opportunity to study large numbers of real-world, power plants time-series datasets under actual real-world exposure conditions becomes an essential scientific resource. This combined with network modeling of the active degradation pathways in the module help guide development of higher performance, longer lifetime PV modules such as the new c-Si PERC modules now entering the market.

We have developed a month-by-month (MbM) time-series analysis method to extract features and performance loss rates (PLR) or rate of change (ROC) from measured power output and time-series I-V curves of PV systems in the field. The month-by-month method consists of 3 modeling steps, first, the β (beta) model, subsets the PV inverter data into 30 day pseudo-month section and determines a model of the power as a function of the given weather conditions. Using satellite-based weather data the weather conditions for each system are applied to each of the β models, producing a predicted power output for each of the 30 day pseudo-months. Second, the ξ (xi) model fits a weighted linear regression or a piecewise linear model to the predicted power values from the β models. The PLR is determined from the slope of the ξ model. Finally, the γ (gamma) model is used to rank the importance of the external variables of the inverters, such as the brand of the module or the Köppen-Geiger climate zone of the PV site, on the PLR of the system.

To determine the active degradation pathways and lifetime of photovoltaic (PV) modules, a statistical learning approach is necessary. Structural Equation Modeling (SEM) allows for exploratory modeling, resulting in a system of equations describing the univariate relationships between variables. However, SEM typically only fits a system of linear equations, so we have developed network SEM (netSEM) that enables nonlinear relationships among variables and is recently released as an R package on CRAN. Applied to indoor accelerated and outdoor exposure tests of PV modules, netSEM also allows for cross-correlation of indoor and outdoor degradation models.

Biography

Roger H. French is the Kyocera Professor of Ceramics in the Case School of Engineering, Case Western Reserve University, Cleveland, Ohio. He has secondary appointments in Macromolecular Science, Biomedical Engineering, and Physics. He is the faculty director of the CWRU Applied Data Science program which offers a minor university-wide. He is the director of the SDLE Research Center at CWRU, an Ohio Third Frontier, Wright Project center focused on lifetime and degradation science of long lived technologies and data science and analytics. Prior to joining Case Western Reserve in 2010, French was a Research Fellow in Central Research and Development, DuPont Co. (starting in 1985) and Adjunct Professor of Materials Science, University of Pennsylvania (from 1994). He received his B. S. from Cornell University and his Ph.D. from Massachusetts Institute of Technology, both in Materials Science.



Using vacuum ultraviolet and optical spectroscopies, spectroscopic ellipsometry, and computational optics, his research is in optical properties, electronic structure, and radiation durability of optical materials, polymers, ceramics, and liquids.

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NICOLA MARZARI

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Computational design and discovery of novel materials

Quantum-mechanical simulations have become massively used tools for scientific discovery and technological advancement: thanks to their predictive power they can suggest, accelerate, or support actual physical experiments. This is a far-reaching paradigm shift, substituting the cost- and time-scales of brick-and-mortar facilities, equipment, and personnel with those, very different, of computing engines, and aiming at understanding, predicting, or designing the properties and performance of novel or complex materials and devices with computer simulations.

I will highlight how the convergence of high-performance computing, high-throughput computing, and data analytics is heralding a revolution in the effort to discover novel materials with improved properties and performance. I will in particular discuss the software infrastructure required to create, monitor, record, reproduce, and disseminate millions of complex calculations, and illustrate its power and promise with an example dedicated to the discovery of novel two-dimensional materials with outstanding electronic, optical, or topological properties.

Biography

Nicola Marzari has a "Laurea" degree in Physics from the University of Trieste (1992), and a PhD in physics from the University of Cambridge (1996). He moved to the US as an NSF postdoctoral fellow (Rutgers University, 1996-98), and then as a research scientist first at the Naval Research Laboratory (1998-99) and Princeton University (1999-01). In 2001, he was named assistant professor in computational material science at the Massachusetts Institute of Technology, where he was promoted to associate professor in 2005, and named Toyota Chair of Materials Engineering in 2009. After 10 years at MIT, Nicola Marzari joined the University of Oxford, as its first Statutory (University) Professor of Materials Modelling, and as Director of the Materials Modeling Laboratory. Nicola Marzari holds the chair of Theory and Simulation of Materials at the École Polytechnique Fédérale de Lausanne, where he is also the director of the Swiss National Centre on Computational Design and Discovery of Novel Materials. Current, he is the chairman of the Psi-k Charity and Board of Trustees.



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MARC MOSCH

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The Material HUB – Novel materials

Novel materials play a decisive role in innovation processes and are the prerequisite for a large number of new products. The location Dresden represents an important European center in the field of materials research with the Excellence University TU Dresden and a large number of non-university institutions. The broad scientific and technological spectrum as well as the enormous research density in combination with a high level of professional networking lead to synergy effects among scientists on the one hand and provide the economy with an enormous locational advantage on the other. If these advantages are to be fully exploited, unified, intuitive access to information is required. Currently, however, material data is typically stored on a large number of separated data sets, some of which have limited access, and is described according to heterogeneous schemes and in varying degrees of detail. Although research portals already exist, they are domain-specific, chargeable or only offer user interfaces tailored to specific target groups, rendering them hardly usable by other users. Distributed searches across multiple data sources and portals are time-consuming and tedious. The integrated materials research platform Material Hub presented here is intended to provide a remedy. It must meet the requirements of manufacturers and suppliers whose data it contains as well as the requirements of users from research, industry and trade. This platform, which integrates the Dresden scientific area, is intended to stimulate further first-class research and innovation achievements, promote cooperation and considerably facilitate the marketing of innovative ideas and solutions.

An important aspect of the Material Hub is the combination of different data sources in a central research portal. It integrates research data, manufacturer information and application examples that are heterogeneous in terms of domain, level of detail and underlying scheme. The speech covers the fundamental ideas as well as scope and status of project and platform.

Biography

Dr.-Ing. Marc Mosch leads the Material Hub project at SLUB Dresden. He is interested in service description and linked open data as well as in data and network protection and security. Before his time at SLUB he applied and extended his expertise in the projects EEembedded at the Institute of Construction Informatics at TU Dresden and within the FlexCloud project at the Chair of Computer Networks at TU Dresden. He received his doctorate in 2014 on the topic “Ensuring Data Sovereignty in the Cloud”, developing a private cloud approach that offers the benefits of public clouds and at the same time eliminates their drawbacks. At SLUB his team strives to develop Material Hub, a portal for free-of-charge and cross-resource access to material data for everyone.



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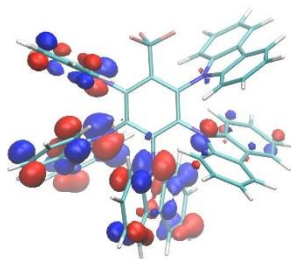
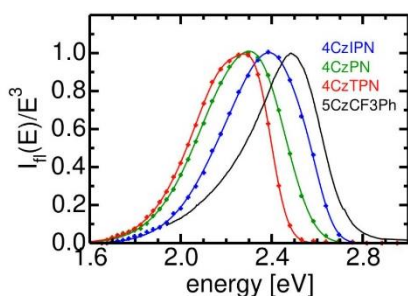
REINHARD SCHOLZ

Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and
Institute for Applied Physics, Technical University of Dresden, Germany

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Thermally activated delayed fluorescence - A new route to more efficient OLEDs?

In molecules with a small splitting between the lowest excited singlet and triplet states, reverse intersystem crossing (RISC) from the triplet to the singlet requires only a small activation energy, resulting in thermally activated delayed fluorescence (TADF). Donor-acceptor (D-A) compounds with large dihedral angle between these subgroups allow for a sufficiently small singlet-triplet splitting of charge transfer transitions, at the price of a reduced transition dipole and a rather slow radiative recombination rate. The present contribution addresses suitable D-A compounds, characterized by an interplay between steric hindrance and decoupling of the frontier orbitals localized mainly either on D or A. In a comparison between time-dependent DFT applying global hybrid functionals, TD-DFT with range separated hybrids, and coupled cluster techniques, it turns out that range separated hybrids reproduce essential results of CC2, at a dramatically reduced computational cost. Applications of some prototypical TADF emitters in blue and white OLEDs reveal present achievements and future challenges for OLED lighting technologies.



Emission spectra of different TADF emitters, and HOMO of 5CzCF3Ph

Biography

Reinhard Scholz studied physics at RWTH Aachen, where he has obtained a doctorate in Condensed Matter Theory in 1992, working on transient optical spectra of inorganic semiconductors. After several research stays at Scuola Normale Superiore (Pisa), TU Chemnitz, TU München, and TU Ilmenau. 2010, he joined TU Dresden, where he is working at the Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP).



His main research interests concern electronic states and spectroscopic properties of organic and inorganic semiconductors together with their applications in optoelectronic devices.

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JÖRG SCHUSTER

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Simulation of Materials, Processes and Devices for Nanoelectronic Engineering

By giving an overview on our activities in the field of computational studies in nanoelectronic engineering, we will contribute an application perspective to the workshop. Advanced fabrication processes are required for the fabrication of leading edge micro- and nanoelectronic devices. The process quality crucially determines the properties of the integrated materials and hence the function of the devices. It will be demonstrated that computational studies along the production chain are valuable tools for process- and device optimization. In addition, simulations are also very useful for the exploration of promising future device concepts and the related novel fabrication processes.

On the way towards predictive simulation of device properties from material properties and their dependence on fabrication processes we will show some first steps. The presented process examples cover the simulation of sputter processes for leading edge CMOS-devices, the simulation of atomic layer deposition as well as an atomistic view on silicon oxidation processes on the nanoscale. Based on silicon nanowire transistors we will demonstrate how device models can be derived from ab initio studies of strained interfaces. Further application examples will be highlighted quickly.

Biography

Dr. Jörg Schuster received his Diploma in Physics (1997) and his PhD (2002) from Chemnitz University of Technology. He works as a senior scientist and group leader at the Fraunhofer Institute for Electronic Nanosystems (ENAS) in Chemnitz, Germany. Recent topics of his research group are process- and equipment simulation for the microelectronics industry and modeling and simulation of micro- and nanoelectronic devices. The application of electronic and atomistic simulation methods in these fields is one of his special research interests. He is author or coauthor of more than 70 publications in international journals and conference proceedings.



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High-throughput computational discovery of novel opto-electronic materials

One of the key challenges in photoelectrochemical water splitting is to identify efficient semiconductors with band gaps of the order of similar to 2 eV to operate as the large-band-gap component in water splitting tandem devices. Here, we address this challenge by extensive computational screening of ternary sulfides followed by synthesis and confirmation of the properties of one of the most promising materials. The screening focusses on materials with ABS(3) composition taking both perovskite and non-perovskite structures into consideration, and the material selection is based on descriptors for thermodynamic stability, light absorption, charge mobility, and defect tolerance. One of the most promising candidates identified is LaYS3. This material was synthesized directly in thin-film form demonstrating its stability, crystal structure, light absorption, and strong photoluminescence. These data confirms its potential applicability in tandem photoelectrochemical devices for hydrogen production.

Biography

Prof. Kristian S. Thygesen earned his PhD degree in Physics from the Technical University of Denmark (DTU) in 2005. After a post doctoral position at Freie University Berlin he returned to DTU where he became Associate Professor in 2010 and leader of the Molecular Electronics group at the Lundbeck Foundation's Center for Atomic-scale Materials Design (CAMD). He was Director of NanoDTU from 2009-2010 and has been Spokesperson for Psi-k working group on Quantum Transport in Nanostructures since 2009. In 2013 he became Professor at the Department of Physics at DTU and in 2015 he became leader of the Section for Computational Atomic-scale Materials Design.



Recently, his research focuses on the development of first-principles methods for the description of ground- and excited state properties of solids and low-dimensional systems. He co-develops the GPAW electronic structure code, and the Computational Materials Repository (<http://c2db.fysik.dtu.dk/>), holds the ERC grant LIMA, and is member of the Center for Nanostructured Graphene (<http://www.cng.dtu.dk>) and the Center for Novel Materials Discovery (<https://www.nomad-coe.eu>)

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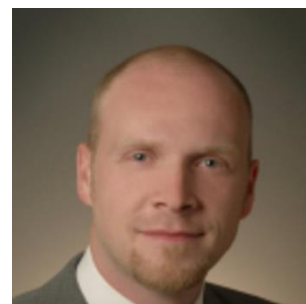
Where no CPU has gone before: GPUs for Deep Learning

Modern Deep Learning training and inference tend to require large computational resources at different ends of the spectrum which current hardware can offer. On top, the software ecosystem has become vast in recent years and choose the right tools can be non-trivial. At the same time, applying deep learning algorithms or extending them is a time consuming effort. So resources should be invested wisely.

With this talk, I would like to give a broad overview on the current lay of the land of benchmarking deep learning applications and frameworks. I will introduce the open-source benchmark deeprace and discuss the insights for single node training and inference obtained so far. The talk will focus on questions like: Are high level frameworks superior to low level frameworks? Are cloud-based resources worth considering or is this just another hype? Is it worth considering multi-gpu training?

Biography

Dr. Peter Steinbach made his Diploma in Physics at the University of Leipzig and went to Dresden for his PhD and wrote about the topic of Experimental Physics. He finished his PhD in the year 2012 and was a research assistant in the institute for Nuclear and Particle Physics at Technical University of Dresden until 2014. Nowadays, he is working as a scientific software engineer for the company Scionics Computer Innovation GmbH.



YOUR NOTES:

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A machine-learning approach for the discovery of novel hard-magnetic phases

High-performance permanent magnets are key materials for environmentally friendly technologies and indispensable for wind turbines and electro mobility. We have carried out a combinatorial high-throughput screening (HTS) approach using density-functional theory calculations in order to identify novel hard magnetic materials with a reduced amount of rare-earth elements. Here, the tight-binding-linear-muffin-tin-atomic-sphere-approximation is applied as a fast DFT method to compute the material parameters that characterize a magnetic material, namely the magnetization M , the anisotropy constant K_1 , and the anisotropy field H_a . Subsequently, we use kernel-based machine-learning (ML) methods to predict optimal chemical compositions for new permanent magnets. For encoding the structural and chemical information of the HTS data in a machine-readable format, we use several existing and newly developed material descriptors and assess the predictive power of the ML models built with them. The accuracy of the ML models with an optimal choice of descriptor and model parameters enables the prediction of promising structure-composition combinations for substitutes of state-of-the-art magnetic materials like Nd₂Fe₁₄B - with similar intrinsic hard-magnetic properties but no or less amounts of critical rare-earth elements.

Biography

Dr. Daniel Urban studied physics in Freiburg and Paris and got his diploma in 2002. Subsequently, he did his PhD on the topic of Stability, Symmetry Breaking and Scaling Properties of Metallic Nanowires and in the field of theoretical mesoscopic solid state physics. In 2006 and after two research stays at the University of Arizona, he received his PhD from the University of Freiburg, where he continued to work as a post-doc. His research touched several aspects of charge and spin transport in nanostructures of one, two or three dimensions and made him move to the Universidad Autonoma de Madrid for some time. In 2012, he joined the group Materials Modeling at the Fraunhofer Institute for Mechanics of Materials in Freiburg which he is now heading since 2017.



For his current research he uses methods based on quantum mechanics or classical atomistic mechanics and on multi-scale materials modeling in order to develop material models and predict physical, chemical, and mechanical material properties.

YOUR NOTES:

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SEYED MEHDI VAEZ ALLAEI

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Phononic heat transport and thermal rectification in low dimensional heterostructures

Manufacturing nanoscale electrical and mechanical devices, as low dimensional heterostructures, has motivated deep understanding of heat transport in low dimensional systems. Specifically, in phonon dominated thermal transport, phonons can be manipulated for controlling heat transport at all temperatures [1], and interesting features similar to thermal rectification can be obtained [2-6]. Due to the different type of interaction between components in heterostructures such as layered media, the transport is more complicated. Here, using molecular dynamics simulations as well as lattice dynamics calculations, asymmetric and anisotropic thermal transport in different 2D and/or layered nanostructures will be discussed. In particular, transport through and across interface, specially in asymmetric layered media [5,7-10], and the important of anisotropy in the structure of 2D systems, e.g. arsenene [11], will be addressed.

Biography

Prof. Vaez Allaei studied Physics at Iran University of Science and Technology from 1994 to 2001. After receiving his master degree, he started his PhD at the Institute for Advanced Studies in Basic Sciences and became a Professor (Assistant) at the Department of Physics at the University of Tehran. He is now an Associate Professor at the University of Tehran for the Department of Physics.

His main research topics are Wave Propagation in Porous Media, Nano Scale Heat Transfer, Surface and Interface Growth, Crack Propagation, Granular Media, Molecular Simulations, Porous Media and Membranes.



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Computational and Experimental Perovskite Redox Materials Design for Solar-Thermochemical Processes

Perovskites and their solid solutions are ideal candidate materials for application in two-step thermochemical cycles. By tuning their redox thermodynamics through composition adjustment, ideal perovskite materials can be designed for each type of application, such as fuels production or air separation. Within this presentation, it is shown how these materials can be designed in silico with the help of density functional theory (DFT) and in the framework of The Materials Project.^[3] In parallel, some of these perovskite materials are synthesized and their thermodynamic data is fit computationally. By creating a model based on theoretical and experimental data, we screened over 240 perovskite solid solutions and added the results to The Materials Project and as a contribution to MPContribs, the user data portal of The Materials Project. By this means, we created a web interface containing user-interactive graphs, which will be made available freely to the public. The web interface is demonstrated and it is shown how materials can be selected with the help of computational methods based on their redox properties. We are convinced that this data helps accelerate the discovery of new redox materials through bypassing the time-consuming search of materials in the laboratory, which is often based on trial and error.

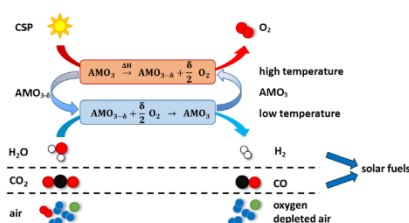


Figure 2: Thermochemical cycles based on AMO_{3-δ} perovskites for the production of solar fuels or for air separation. Adapted from [1,2].

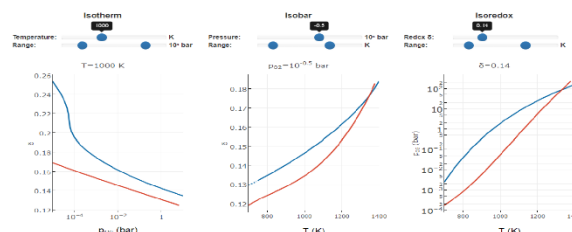


Figure 1: User-interactive graphs describing the reduction of a (Ca,Sr)(Mn,Fe) perovskite oxide based on its thermodynamics according to theoretical data (red) and experimental data (blue).

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Biography

Josua Vieten is working on his dissertation at the Institute of Solar Research of the German Aerospace Center (DLR). His research is focused on the targeted design of perovskite redox materials for solar-thermochemical processes. In fall 2017, he worked as a visiting researcher at the Lawrence Berkeley National Laboratory (USA). He received a master's degree in Chemistry from the TU Munich in 2016 and a master's degree in Advanced Materials Science from a joint program of TU and LMU Munich and the University of Augsburg in 2015.



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CONTRIBUTED TALKS

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Design of bio-inspired materials: Emerging innovation from deep learning

Accidental and deliberate extreme loads on civil and military structures, locally and internationally have claimed lives and cost governments billions of dollars worldwide. This poses challenges to develop a high performance protective material that exhibits superior strength and toughness simultaneously.

Engineered composite materials are widely used to create adjustable materials to achieve superior performance in protective engineering applications. However, traditional engineered materials typically exhibit inherent conflict between strength and toughness. Natural materials, which possess high strength without sacrificing toughness via the hierarchical composition of hard and soft phases, are a key innovation to design high performance materials. Hard materials normally possess high strength but fail suddenly in the presence of cracks, whilst incorporating soft phases into hard materials can alleviate stress concentrations and crack propagation, thereby resulting in stronger and tougher composite materials. However, searching for the optimal design of such composite material is challenging due to the large number of possibilities, thereby making it difficult to achieve by an exhaustive approach.

Deep learning is the cutting edge of Artificial Intelligence in computer and data science, which allows computers to learn, predict and optimise new materials. The paper proposes an intelligent material design framework based on a new deep learning model for designing bio-inspired materials. The deep learning model is able to generate an optimal design, which inclusively maximises the strength and toughness of the material, at a much lower computational cost compared to an exhaustive approach. Computational simulations will be used to generate training data for the intelligent material design framework. The results show that the deep learning framework can search for an optimal design, which is better than the mean properties of the input training data. The proof-of-concept will be validated by using advanced manufacturing to fabricate the intelligent bio-inspired material in this study.

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Bayesian Optimization to Model Polymorphism and Phase Transition Mechanisms in Small Molecule Organic Semiconductors

Organic electronics have made significant headway in commercial products, most notably, the colorfully bright displays of mobile devices that are based on organic light-emitting diodes. This increased interest in organic electronics is primarily due to the advantages they offer in terms of unique properties such as flexibility, stretchability, and low-cost manufacturing over conventional materials, primarily silicon-dominated, in the electronics industry. However, a major difficulty in deploying organic semiconductors is their predilection to pack into multiple, structurally distinct, crystal structures (polymorphism) with differing ability to transport charge. For example, di-tert-butyl[1]benzothieno[3,2-b][1]benzothiophene (ditBu-BTBT) is an organic semiconductor which exhibits remarkably high mobilities, $\sim 7.1 \text{ cm}^2/\text{Vs}$. A BTBT variant, diTMS-BTBT, which features bulkier side groups, is another high performing p-type organic semiconductor, but both these molecules have been shown by the Diao group at UIUC to exhibit polymorphic behavior.

Controlling polymorphism is critically important since even slight variations in π -orbital overlap can lead to orders of magnitude difference in charge carrier mobility. Very few studies exist that investigate the origin of polymorphism and mechanism(s) for transitions among polymorphs. Major challenges are the low energy barriers between polymorphs (O(meV)), ultrafast kinetics, and structural reversibility. A deeper understanding of the processes involved might open the door for stabilizing metastable polymorphs for structure and charge transport studies. To study these polymorphs, we conducted a detailed computational study to predict the structures of stable and metastable polymorphs, and understand inter-polymorph phase transitions in BTBT systems. While experiments have only found two polymorphs, molecular simulation is capable of identifying all the thermodynamically and kinetically stabilized polymorphs.

Finding the optimal energy structures is non-intuitive and involves iteratively choosing the chemical structure, composition, or processing conditions to synthesize new materials, and improve on the design by testing their physical properties until exhaustion is achieved. For polymorphs, this "materials discovery" task requires finding the best combinations of a candidate's six dimensions of unit cell lengths and angles and temperature that lead to the lowest energy structure. Employing an iterative Edisonian approach is wasteful (and usually impractical) in terms of synthesis time, effort, and resources. We have addressed this issue by incorporating Bayesian Optimization (BO), a Machine Learning (ML) technique, into Molecular Dynamics (MD) simulations to predict the structures of thermodynamically stable and metastable polymorphs. Our novel approach is intended to uncover the relationship between structure and materials properties, in our case, minimizing the total energy as a function of the design parameter, essentially our objective function (or metric for success), and uses decision theory to guide the choice of experiments during material design in such a way that we minimize the number of experiments we need to conduct to get to an optimal solution (driven by the objective function), while still retaining the fundamental physics of the problem. Combining MD and BO allowed us to predict the total energy as a function of the spatial arrangement of atoms inside the crystal, and identify the energy-minimized optimal structures obtained by running time-consuming, expensive molecular simulations for only a small fraction (~ 15 -20 percent) of the entire set of possible candidates (over 1000 structures).

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Smart nanometrology with Machine Learning

Over the last decades, there has been increasing use of Artificial Intelligence (AI) tools over many technological areas bearing a great impact on society. The recent growth of semiconductor market has been focusing on applying these AI tools and specifically Machine Learning (ML) models to solve problems regarding to more advanced and faster chips and applying more intelligent data analysis ^[1]. Software tools used by ML techniques could add value to complex nanomanufacturing process, enabling more efficient handling of data, making better decisions and interferences.

Nanomanufacturing contains a lot of sub-processes and every one of them is characterized by a set of parameters. The three main sub-process are nanofabrication, nanometrology and nanofunctionality. Nanofabrication is responsible for designing and constructing the nanosurface. After the nano-surface is constructed another set of parameters must be measured to characterize its structure (topography, roughness etc.) and that is a part of Nanometrology. The last part of the nanomanufacturing process is the nanofunctionality. This step involves parameters related to the final properties of the nanostructure where nanofabrication aimed from the start (properties like superhydrophobicity, resistivity, light reflection, chip performance etc.).

Evaluating every process consumes time and resources. Industries that use relative manufacturing steps cannot use these techniques on every product they make. ML tools can assist this process by making predictions and extract features that are important to every individual process offering useful information ^[3]. That information can be used to give us experience and understand better which parameters are more significant for the next or previous process.

The thesis motivation is coming from the large number of roughness parameters proposed and used for the characterization of nanosurface, which however are calculated with no reference to the targeted application ^{[4],[5]}. Industry and science often encounter many of them that can describe the nanometrological parameters with regards to the specific functionality creating a parameter proliferation. The aim of this thesis is to create ML models that step between the manufacturing process of rough nanostructures and connect their nanofabrication parameters to the nanometrological ones while also extracting internal features. More specifically, we focus on the active area of a rough surface, which affects surface functionality in many applications, and seek its dependence on the first moments of height distribution (rms, skewness, kurtosis) as well as surface anisotropy and lateral correlation length.

We create high resolution simulated surfaces by a choosing the specific roughness parameters and investigating theirs on the active area of surfaces. By creating different types of surfaces with a variety of input parameters a database is finally created which a part of it will be chosen to train our ML model. More specifically, we train deep feed forward back-propagation neural networks and random forest model. A part of the database is left for testing the model and validating the training method (k-fold cross validation). After the model is created it will be investigated to extract features based on the weights that were assigned during training.

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POSTERS

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Size Influence on the Relative Stability of Trigonal Prismatic and Octahedral Phases of MoSe₂ Nanoflakes

Two-dimensional transition metal dichalcogenides (TMDs), MQ₂ (M = transition metal; Q = S, Se, Te), have attracted great attention due to their unique properties and several promising applications [1,2]. Each TMD layer is composed of one plane of M atoms sandwiched between two planes of Q atoms, and a polymorphism arises from a variety of coordination environments, trigonal prismatic, octahedral and distorted octahedral [1,3]. Several factors that affect chalcogenides properties have been identified, such as variation of number of layers [4] and composition [5,6], and the differences between the properties of TMDs polymorphs [1,3] allows a strategy to tune the properties of TMDs. Therefore, there is great interest in understanding and controlling the relative stability between the structural phases of TMDs [3]. We performed a density functional theory investigation of the relative stability of trigonal prismatic and octahedral (MoSe₂)_n nanoflakes, with *n* ranging from 15 to 192. We found that the octahedral phase has an energetic preference for the distorted configuration, due to a Peierls transition mechanism demonstrated for MoSe₂ monolayers, whereas the structural configuration in the core of trigonal prismatic nanoflakes is preserved, and the M terminated edges exhibit a strong reconstruction pattern. From the calculated relative total energy between the nanoflakes we show that the nanoflake size has an important effect on the relative stability between the two phases. The octahedral phase is energetically favored for the smallest nanoflakes, but with the increase of size the lowest energy polymorph becomes the trigonal prismatic, which is the ground state phase in bulk and monolayer MoSe₂.

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Application of 2D materials as anode materials for advanced Na or Li ion-batteries

Rechargeable metal-ion batteries now-a-days play a pivotal role in modern transport, communication and electronic industries. A common commercial anode electrode material, graphite is highly stable, nonetheless, it not only suffers from a moderate charge capacity of 372 mAh/g, but also the ions diffusion are not fast enough and therefore the need of replacement with another anode material is inevitable in order to satisfy the quickly growing market. During the last decade, various bulk materials like silicon have been probed as anode electrodes to improve the performance of metal-ion batteries, however the practical successes have not been considerable due to several technical issues such as degradation. Since two dimensional (2D) materials and their heterostructures exhibit good stability, extensive adsorption energy, fast ion diffusions and high storage capacity due to their great surface to volume ratio, they have progressively attracted attentions for the application as electrodes in high performance rechargeable batteries. In this work, we employ first-principles density functional theory calculations to investigate the interaction of Na or Li atoms with single-layer and free-standing 2D films such as borophene, graphyne, silicene, germane, stanene and vanadium dichalcogenides. In our modelling, first the strongest binding sites were predicted and next we gradually increased the adatoms concentration until the maximum capacity was reached. Bader charge analysis was employed to evaluate the charge transfer between the adatoms and the borophene films. Nudged elastic band method was also utilized to probe the ions diffusions. We calculated the average atom adsorption energies and open-circuit voltage profiles as a function of adatoms concentrations. Our study provides useful viewpoint with respect to the future application of 2D nanomembranes for the design of high capacity and light weight advanced rechargeable ion batteries.

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Numerical investigation of an artificial neural network based identification of nonlinear material parameters

This work is concerned with determining material parameters in the incompressible hyperelastic materials namely Mooney-Rivlin and Yeoh materials. Firstly, Linear Regression on Tensorflow framework used as a curve fitting method for synthetic data produced from the equation of the first Piola-Kirchhoff stress tensor of the uniaxial tension, biaxial tension. The result parameters from the Linear Regression are identical with that of synthetic data with an appropriate error. Secondly, the second curve fitting approach is introduced using the Artificial Neural Network for the same task and compared the performance with the previous one. Finally, the classical experiments of Treloar and Jones and Treloar on natural rubber data is the subject for validating the performance of the curve fitting methods, the result materials constants are expected to fit well with the validation data.

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Dopant driven electronic and energetic changes in Li-ion battery positive electrode materials from first-principles

LiNi_{1-y-z}CoyMnzO₂ (NCM) and LiNi_{1-y-z}CoyAlzO₂ (NCA) are now the most common positive electrode materials for lithium intercalation batteries. But with Co contents of up to 20 %, the rising cost and limited availability of Co could prove prohibitive to giga-scale production. Here, using first-principles calculations, we examine how Al, Mn and other substituents change the electronic structure and energetics of model Ni-rich positive electrode materials. Specifically, local changes in charge density and densities of states are connected to changes in oxygen chemical potential and lithium intercalation energy. This furthers fundamental understanding of nickel-rich positive electrode materials and serves to point the way to new chemistries that are safe, lower-cost, and with minimal energy density sacrifice.

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Temperature dependent optical constants of noble metals Au and Ag

In recent years, metallic nanoparticles have been exploited as nanoscale converters of electromagnetic energy into heat. This approach has the advantage of providing heat on a very local scale, in a remotely controllable way and possibly on an ultrafast time scale. This can be very useful for biomedical applications, such as local hyperthermia and for other applications, such as heat-assisted magnetic recording ^[1]. The presence of a Localized Surface Plasmon Resonance (LSPR) provides an extra degree of freedom in tailoring the optical absorption of nanoparticles with respect to the material's bulk counterparts. For this reason, the noble metals Au and Ag are the most widely exploited for thermoplasmonics. In order to model the thermo-optical response of metal nanoparticles, it is necessary to know in detail the dielectric function of the constituent materials as a function of temperature. Here, we present a study of the temperature dependence of the dielectric function of Au and Ag optical thick films deposited by means of Molecular Beam Epitaxy in UHV ($P=10^{-9}$ mbar). The investigation was performed by spectroscopic ellipsometry (SE) under high-vacuum conditions ($P=10^{-7}$ mbar), employing a portable roll-on/roll-off vacuum chamber set within the arms of a J.A. Woolam M-2000 ellipsometer ^[2]. The investigated temperature range is between room temperature and 623 K; the optical spectral range is 245-1700 nm. As a function of increasing temperature we observe definite changes in the dielectric function of the metals. In the case of Au, we can notice both a broadening of the interband transitions and a significant increase of the intraband contribution (so called Drude tail). In the case of Ag, interestingly, we observe that an absorption peak in the 310-350 nm wavelength range progressively splits off from the interband transitions, while in the free electron region the changes are less marked. The extra-peak which appears at energies just below the so called X-point must be kept into account in thermoplasmonics measurements/modelling as it directly affects the Ag LSPR spectral range ^[3]. Our data show that accurately evaluating the temperature dependence of the dielectric function is mandatory to correctly model the thermo-optical properties of metallic nanoparticles systems.

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Image-based size determination of agglomerated particles via convolutional neural networks

The properties of nanomaterials (e.g. mechanical, optical, catalytic, biological, etc.) are determined by their characteristic length as well as their shape ^[1]. In case of nanoparticles, the characteristic length is usually some kind of equivalent diameter (e.g. hydrodynamic, volume-based, surface-based, etc.) ^[2]. There are various techniques available for the determination of the different types of equivalent diameters, one of them being electron microscopy (EM) ^[3]. The determination of particle size distributions (PSDs) of non-agglomerated particles on TEM images can already be performed partially or fully automated since several decades ^[4]. By contrast, the determination of PSDs of agglomerated particles still depends on the recognition of primary particles by a human operator. This practice is not only laborious, expensive and repetitive but also error-prone due to the subjectivity and exhaustion of the operator ^[5]. To solve this problem, new approaches to imaging particle analysis, with help of convolutional neural networks (CNNs), were proposed, implemented and validated. CNNs were used for the preprocessing (denoising and deblurring) as well as the classification (i.e. shape identification) and semantic segmentation of agglomerated particles on various kinds of electron microscope images. A major challenge of the proposed method is the fact that the training of CNNs requires up to several hundreds of thousands of samples with known properties to avoid overfitting ^[6], i.e. that the CNNs are not able to generalize when being confronted with previously unknown data. Unfortunately, there is no publicly available source of already evaluated samples and a manual evaluation of such a large number of images is hardly feasible, due to the reasons that were given before. Therefore, EM images with defined characteristics were synthesized and used for the training of the CNNs. For an effective training, the lifelikeness of the synthesized images is of utmost importance. Finally, the CNNs were validated based on real samples, to prove their usability in real-life applications. To speed up the image synthesis as well as the training of the CNNs the necessary calculations were performed on graphics processing units (GPUs), whenever possible.

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Plasmonic Molecular Switches: A Computational Approach to Explore Light-Matter Interaction at a Quantum Scale

Quantum plasmonics, a fascinating combination between plasmonics and quantum optics, is an emerging field arisen from the interest of the scientific community to study at a quantum level the interaction between light and matter at the nanoscale. During the past decades, plasmonics has largely demonstrated, through numerical simulations based on classical electromagnetism [1] and a wide range of applications [2], the possibility to confine the electromagnetic fields to regions well below the diffraction limit. These developments have been made possible thanks to the incredible progress on both the nanoscale fabrication techniques and powerful electromagnetic simulations. On the other hand, the quasi-particle nature of plasmons, makes plasmonics an intriguing field also from a fundamental point of view, with the opportunity to explore the arena of quantum effects naturally appearing when the systems of interest are scaled down to a sub-nanometer range. Anyway, once we enter the quantum regime of interaction at the nanoscale, we have to face the problem that classical predictions based on the Maxwell's laws fail in the description of the effective surface charge induced by the incident electromagnetic field. Consequently, to take into account the intrinsic atomistic structure of matter, a quantum mechanical based approach becomes mandatory. Here, I propose a Time Dependent Density Functional Tight-Binding [3][4] study on the physics of interaction in a hybrid metal-molecule system, which could provide a proof-of-concept of a plasmonic molecular switch. The hybrid system analyzed is composed by a plasmonic part, a tetrahedral cluster of 20 silver atoms, and by a molecular part, a stilbene molecule functionalized with a benzene ring and a COOH group. In more detail, stilbene belongs to a particular kind of molecules, named molecular photoswitches, that can change reversibly their spatial conformation (passing from a cis-state to a trans-state and vice versa) interacting with a particular wavelength of light. This mechanism is called photoisomerization process. Here, we are interested to the possibility to use this process to optically control and tune the plasmonic response of a nanostructure. The analyzed system seems to give an optimistic chance for the future developments of optoelectronics, facing the theoretical challenge of a tunable/switchable response in plasmonic systems at a quantum regime of interaction. In a visionary outlook, this could represent an important step towards a new generation of quantum technologies for information processing and computing [5], at the crossroads of plasmonic and molecular electronics.

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SEM Imaging Beyond Grey Values: Towards Nano-Scale Phase Identification via Machine Learning Applied to Spatially Resolved Electron Spectra

Many recent developments in materials science are facilitated by sophisticated organic-inorganic hybrid nanomaterials or nanostructures. Examples are zeolites, metal organic frameworks, 3D scaffolds from additive manufacturing, organic-inorganic perovskites and organic photovoltaic blends. Performances of these materials rely on complex interfacial effects and defects, which is why direct nanoscale visualization is typically inevitable for their understanding and optimization. Electron microscopy is frequently used here since it exclusively features the combination of the required (sub-) nanometer resolution with a variety of spectroscopic methods, offering information beyond conventional contrast mechanisms. It was for example demonstrated ^[1] that effective nanoscale phase identification in organic photovoltaic blends can be realized by applying supervised non-linear manifold learning to spatially resolved electron energy loss datasets from transmission electron microscopy (TEM). However, the organic semiconductors used as well as many other functional materials for nanotechnology are highly sensitive to beam damage. It is commonly accepted that beam damage can be reduced by strongly decreasing the primary energy of the incident beam electrons, total electron dose and dose rate.

A novel prototype of an aberration-corrected ultra-low voltage scanning electron microscope (ULV-SEM), the Zeiss DELTA®, allows for lowering the primary electron energies down to 20 eV, while maintaining high resolution. Such low landing energies, instead of typically ≥ 1 keV in SEM and 20 kV to 300 keV in TEM, are expected to drastically reduce beam damage or limit it to a very small volume. Furthermore, a dedicated energy filter allows the generation of spatially resolved electron spectra by successively varying an upstream voltage for the emitted secondary and backscattered electrons. Unfortunately, no physical models exist to predict or evaluate the corresponding spectra in the ultra-low voltage regime. Analysis of the spectra is additionally complicated by noise and their convolution with an unknown device response function. Instead of developing dedicated physical models and deploying a complex and technically challenging device characterization, we demonstrate how nanoscale phase identification can be achieved by applying machine learning algorithms to spatially resolved electron spectra. The goal is to identify physically meaningful parameters and separate them from interfering device signals. Preliminary results show the detection of subtle features in secondary electron spectra of well-known donor-acceptor organic photovoltaic blends by unsupervised non-linear manifold learning. The derived phase discrimination is in agreement with results from spectroscopic TEM measurements as described in ref. 1. We expect that robust workflows combining multidimensional data from the ULV-SEM and multivariate statistical data analysis will enable seminal structure-property investigations on materials for energy, nanomanufacturing, and catalysis applications.

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Graphyne-3 as a Membrane for Separation of CH₄/ CO₂ Gas Mixture

Graphyne-3 sheet, a carbon-based structure which has intrinsic nanoscaled pores is used as a membrane for separating CH₄/CO₂ gas mixture by the method all-atom molecular dynamics simulation. In a constant pressure difference between the two sides of the membrane, it is found that the flux of CO₂ is three times larger than the flux of CH₄ in an initially equimolar mixture, and this ratio is found to be three times of the ratio of initial number of molecules for different initial ratio concentrations. So graphyne-3 is a good choice for CO₂ extraction. It is shown that the linear shape of CO₂ helps it to permeate faster, in which it can be seen that the CO₂ tends to permeate perpendicularly to the graphyne surface which minimize the interaction energy between that and graphyne. Also it is shown that we have to pay attention to the adsorption of CO₂ to the graphyne membrane, which it is shown that a layer is made by CO₂ molecules which will lower the efficiency through time.

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High throughput molecular dynamics calculations of cations motions in hybrid perovskites

Hybrid halide perovskites have taken the spotlight of photovoltaic materials research over the past decade. Solar cells based on these materials have already crossed the maximum device efficiency of 22%, comparable to crystalline silicon. Although the material has a simple ABX_3 stoichiometry and corresponding structure, it also exhibits dynamic processes that significantly affect material properties. The organic cation A^+ offers not just structural stability and charge neutrality to the BX_3 --- but has also been shown to affect the mobility of charge carriers. The A^+ is dipolar and influences the electronic properties by its ability to reorient. The non---zero electric field created by the interacting dipoles leads to domains of high and low electrostatic potential. We study the reorientation of the cations by molecular dynamics simulations in which we show how the cations movement is affected by temperature and how does this is connected to the change in crystal structure that occurs at low temperature. To perform these calculations, we have taken a super cell of $10 \times 10 \times 10$ unit cells. The calculations were performed with periodic boundary conditions. To compare our results for a specific dipole moment we have performed similar calculations with low the low---dipole moment organic cations formamidinium and validated that it is indeed the dipole moment of the cation that is responsible for the observed structural change.

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An Accelerated Metal-Semiconductor Classification of Functionalized MXene using Machine Learning

With the aim to revolutionizes the electronic industries, development of nanoscale devices has led the search for novel two-dimensional (2D) materials with multifunctionality. One such promising candidate is transition metal carbides and nitrides known as MXene, which is exfoliated form corresponding bulk MAX phase. During the exfoliation process, the surface of MXene gets functionalized by the different functional group due to the presence of unsaturated surface charges. The choice of the functional group varies with chemical environment of exfoliation. Hence, an enormous number of MXenes can be generated, which makes the search of a MXene for targeted applications extremely time-consuming. A total of 23,870 MXenes are generated and stored in a functional materials database named “aNANt”^[1]. To have a hold on materials properties, their electronic characterization is essential. However, classifying the metal and semiconductor MXenes by calculating their band gap for such large database by computational technique would be a herculean task. Statics based machine learning has been a promising tool for prediction of materials properties and discovery of new materials at a larger scale. Hence, without calculating the band gap for whole database, we have developed a machine learning model to classify the metallic and semiconducting MXenes. The established model utilizes the elemental properties of the constituent elements of MXene, extracted from known chemical repositories as features or descriptors. The model developed using the various approach such as KNN, bagging and SVM resulted in almost similar performance. With optimized hyperparameters, bagging based machine learning model is able to classify the metal and semiconductor MXenes with an accuracy of 98%, having a large area under the ROC curve. Our model can classify the MXenes in a very efficient way, which significantly reduces the computational cast over calculating band gap of individuals.

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Damage investigations of concrete under impact load using laminography

We examine the behavior of reinforced concrete components subjected to impact induced loading conditions which might be caused by vessels collisions, such as aircraft fuel tanks. The concrete plates were impact damaged at TU Dresden and shipped to BAM. At BAM laminar tomography as the imaging method is used to determine and quantify the damage state. An automatic crack detection method based on template matching is applied to find the cracks and we aim to develop a new method using machine learning Algorithms. In addition, numerical models are developed to understand the experiment and to predict the damage structures based on failure mechanisms.

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Interlaminar reinforcement of carbon fiber composites aligned carbon nanotubes

Aligned nanoscale fibers (carbon nanotubes, CNTs) are used to reinforce the interlaminar resin-rich region of aerospace-grade unidirectional carbon fiber laminates in an architecture termed “nanostitching”. Nanostitching leads to a hybrid architecture where aligned CNTs (A-CNTs) are integrated at the interface of Carbon Fiber Reinforced Plastic (CFRP) plies. Here we manufacture nanostitched laminates and investigate the effect on laminate strength through ex situ and in situ mechanical testing. Short beam shear (SBS) and double edge notched tensile testing were conducted on both baseline and A-CNT reinforced laminates. No statistically significant change was found in SBS strength, however, a ~9% increase in tensile strength was observed in the double edge notched tensile tests. In situ tensile testing of the same double-edge notch configuration utilizing synchrotron radiation computed tomography (SRCT) showed little difference in damage accumulation between baseline and A-CNT reinforced laminates at 80% of failure stress, likely due to a general absence of delamination damage. Future work will focus on acquiring data at stress levels closer to ultimate failure in the double-edge notch configuration, testing configurations that exhibit delamination formation and growth in the damage progression, and improving preliminary modeling (results presented herein) to improve understanding of the different mechanisms at work.

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Physical insights into the operation of a 1-nm gate length transistor based on MoS₂ with metallic carbon nanotube gate

Low-dimensional materials such as layered semiconductors or carbon nanotubes (CNTs) have been attracting increasing attention in the last decades due to their inherent scaling properties, which become fundamental to sustain the scaling in electronic devices. Inspired by recent experimental results (Desai et al., 2016), in this work we examined the performance of MoS₂-channel Field Effect Transistors with 1-nm gate length by means of quantum transport simulations based on Poisson equation and Non-equilibrium Greens function formalism. We considered uniformly scaled devices, with channel lengths ranging from 5 to 20 nm controlled by a cylindrical gate with a 1-nm diameter, as would be required in realistic integrated circuits. Moreover, we also evaluated the effect of the finite density of states of a carbon nanotube gate on the loss of device performance. We noticed that the subthreshold swing for all short-channel structures was greater than the ideal 60 mV/decade limit of thermionic devices and we attributed this to the presence of tunneling currents and gate-drain interactions. We tailored the transistor architecture in order to improve the gate control. We concluded that the limited CNT-channel capacitive coupling poses severe limitations on the operation and thus exploitation of the device.

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Thermal transport in carbon-nitride 2D nanostructures: A molecular dynamics study

Carbon-nitride 2D nanostructures have non-zero electronic energy band-gap (~ 2 eV) in contrast to mono-elemental 2D structures such as Graphene, Silicene, Germanen and Stanene. This brilliant property of carbon-nitride 2D nanostructures make them good candidates for future applications in electronic devices such as transistors or optic diodes. In this study, we calculate the thermal conductivities of four carbon-nitride 2D nanostructures as C2N, C3N, T-NC and T2-NC by performing equilibrium molecular dynamics simulations. Then by simulating carbon-nitride 2D nanostructures inserted on a silica substrate, we report the interfacial thermal conductance using transient molecular dynamics method inspired from the experimental pump-probe technique. Interestingly, we found that despite large difference between the thermal conductivities of carbonnitride 2D nanostructures, their interfacial thermal conductance values with silica substrate is at the same level of magnitude. The results of this study can help to understand the thermal behaviour of carbon-nitride 2D nanostructures with application in nanoelectronics.

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Combinatorial screening optimization of organic solar cells

Organic photovoltaics (OPV) constitute a promising energy technology that currently offers power conversion efficiencies exceeding 13%. OPV is also attracting an increasing interest due to its potential low-cost manufacture in roll-to-roll setups, flexibility, versatility and ease of integration due to their intrinsic lightweight and colour tuning capabilities.

The active layer in the organic solar cells consists of a blend of an electron transporting conjugated small molecule (acceptor) and a hole transporting conjugated polymer (donor) that are blended to form the so-called bulk heterojunction. Both the thickness of the active layer and the blending ratio of the materials have a large impact on the device performance; they mainly determine the fraction of light that is absorbed as well as how well the photogenerated free carriers are extracted.

Recently, we have developed and implemented a combinatorial screening methodology that aims at substituting the usual discrete, sample-by-sample procedure followed in the optimization of these devices. The method is based on the use of lateral thickness and composition gradients in a single device in combination with local photocurrent mapping and Raman imaging to quickly determine the sweet spot in the parameters involved (thickness and blending ratio).

By moving from a fabrication-intensive to a measuring-intensive optimization protocol we demonstrate that the savings in terms of time and resources can be tenths of times higher than those employed in sample-by-sample optimization routines.

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Materials and data analysis: a brief summary

Although data-driven materials science seems to be an emerging field, it lies on solid pillars, constructed since almost thirty years. One of the first aim of such field was to reduce scientists' trust on a trial-and-error approach, allowing a deeper study and comprehension of different materials mechanical, electronic, optical and magnetic properties: simulations and quantum mechanics computation captured scientific world attention when, in 1998, Walter Kohn was awarded the Nobel Prize in Chemistry for his studies on Density Functional Theory [1]. Since then, enormous efforts have been taken in order to please the world's need of new materials, chasing reduction of production costs and ecological sustainability.

In fact, thanks to huge amounts of data, it is possible to discover the relationships between processing parameters, environmental conditions, lifetime characteristics, and many other important factors which can improve research and development on materials [2]. Data collections are intensively analysed in order to find hidden trends which may reveal some specific material property (Figure 1). However, there are still some critical points, for example the lack in the materials science community of data standards which would make easier the process of sharing and collecting data, allowing scientists from different parts of the world to perform parallel research. Nevertheless, there exists an important european project called Novel Materials Discovery Laboratory (NO- MAD), which includes an encyclopedia and various data-analytics tools for materials exploration and discover.

The research in data analysis is strongly based on cutting-edge topics and technologies, such as machine learning. One clear example of this technology potentiality is the astonishing result obtained in 2017 by Google Deepmind's Alphazero, a computer program which has been able to reach a super-human level of play in chess in few hours, only by self-learning, starting from zero knowledge [3]. Before the Information Technology revolution, many scientific achievements could not be reached, or even thought, but new ideas and technology have provided some useful instruments which will be fundamental in materials science development..

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Theoretical Framework for the Computational Study of Hot Electron Generation in Metal Nanoparticles

Solar energy harvesting, be it through photovoltaics or photocatalysis, is of global interest for researchers and the wider society alike. In pursuit of devices with higher conversion efficiencies, the study of new materials is conducted in parallel with the exploration of supporting strategies. One promising approach to enhance photovoltaic conversion consists in using plasmonic nanoparticles embedded in solar cells. These nanoparticles can increase the total light conversion in the device through different processes, but the emphasis of this presentation will be placed on the injection of charge carriers, excited inside the plasmonic nanoparticle, into a neighboring material. In photovoltaic devices, the highly energetic (hot) electrons need to acquire enough energy to traverse the Schottky barrier between metal nanoparticle and semiconductor, thus contributing to the overall generated photocurrent. Importantly, plasmonic resonances couple strongly with light, offering a high absorption cross section, and they can be spectrally tuned through selection of the material composition and geometry of their supporting nanoparticles. This offers the possibility of targeting photon energies lower than the semiconductor bandgap, effectively extending the operative spectrum of the device.

During this talk I will describe a theoretical framework based on a phenomenological account of the hot electron generation process. The model relies on solving the kinetic equation of motion for the electronic density matrix inside a metal nanoparticle, under continuous illumination. One key property of the approach is the inclusion of two different timescales to model the carrier relaxation. This formalism allows the study of relatively large nanoparticles without committing large computational resources and provides a way to integrate it with classical electrodynamic calculations, thus allowing to explore the effect of material composition, nanoparticle geometry and interparticle interaction in the generation of hot electrons. These features make it a useful tool to design plasmonic nanoparticles that successfully enhance light conversion efficiencies in photovoltaic and photosensing devices, as well as photocatalytic systems.

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Identifying the active site in Cobalt mixed oxides for a sustainable energy conversion

The purpose of this work is the evaluation of cobalt atoms in different oxygen coordination towards their activity for oxygen evolution reaction (OER).^[1;2] To produce H₂ from H₂O, the overpotential of the O₂ formation has to be lowered. The best catalysts known are based on iridium and ruthenium oxides. Those expensive metals could be replaced by cheap and abundant first row transition metals as cobalt, and today's research aims to find and create stable and highly active structures among their compounds.^[3]

In addition, when the active site is identified, already existing cobalt-based catalysts could be improved, and the total amount of cobalt could be reduced by tailoring materials with only active cobalt sites. Hence, we synthesized mixed oxide nanoparticles with cobalt only present in either tetrahedral or octahedral oxygen environment. As a reference, we used a material which contains both sites.

The nanomaterials' phase purity and morphology were validated by powder X-ray diffraction (XRD) and transmission electron microscopy (TEM). Local cobalt environment was confirmed by X-ray absorption fine structure (XAFS). A rotating disk electrode (RDE) setup using a glassy carbon electrode was utilized to test the electrochemical performance towards the OER. For all samples, the oxidation of Co³⁺ to Co⁴⁺ could be observed in the range of 1.3 to 1.6 V vs. RHE. As Co⁴⁺ is known to be the catalytically active oxidation state, all samples show activity towards the OER.^[4] Giving an overpotential nearly 100 mV smaller, one site is clearly superior to the other.

Characterizing the different materials thoroughly, we could successfully identify one cobalt oxygen environment to be significant more active towards the OER.

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Strategy to improve lattice mismatch of nickel based superalloy

The lattice mismatch data, containing component, solution treatment, and aging treatment, is collected to develop multivariate regression model. We had some work that composition content made standardization treatment, and the formulation of heating and cooling translated into numerical value to make data set reasonable. Using MATLAB built multivariate regression model and got confidence interval $[-\varepsilon, +\varepsilon]$, with ε is 0.153. With leave-one-out cross validation acquiring the model's weight value 1.32, the result proves that model stability is well. From the result of the lattice mismatch model, it is proposed that the influence proportion during γ' precipitates, and put a strategy to improve lattice mismatch of nickel based superalloy.