

# Hands-on Workshop Density-Functional Theory and Beyond

High-Throughput Screening and Big-Data Analytics,  
Towards Exascale Computational Materials Science

---

---



## Meeting booklet

Barcelona, Spain  
August 26 - September 06, 2019

### Organizers:

Eliseo Ruiz Sabin, Sebastian Kokott,  
Jordi Cirera, Volker Blum, Silvia Chellini,  
Carsten Baldauf, Francesc Illas Riera, Matthias Scheffler

# Contents

<b>1</b>	<b>Practical information</b>	<b>1</b>
<b>2</b>	<b>Program</b>	<b>4</b>
<b>3</b>	<b>Poster Abstracts</b>	<b>8</b>
<b>4</b>	<b>List of Participants</b>	<b>66</b>

**Organized by:**



UNIVERSITAT DE  
BARCELONA



FRITZ-HABER-INSTITUT  
MAX-PLANCK-GESELLSCHAFT

**Endorsed by:**



# 1 Practical information

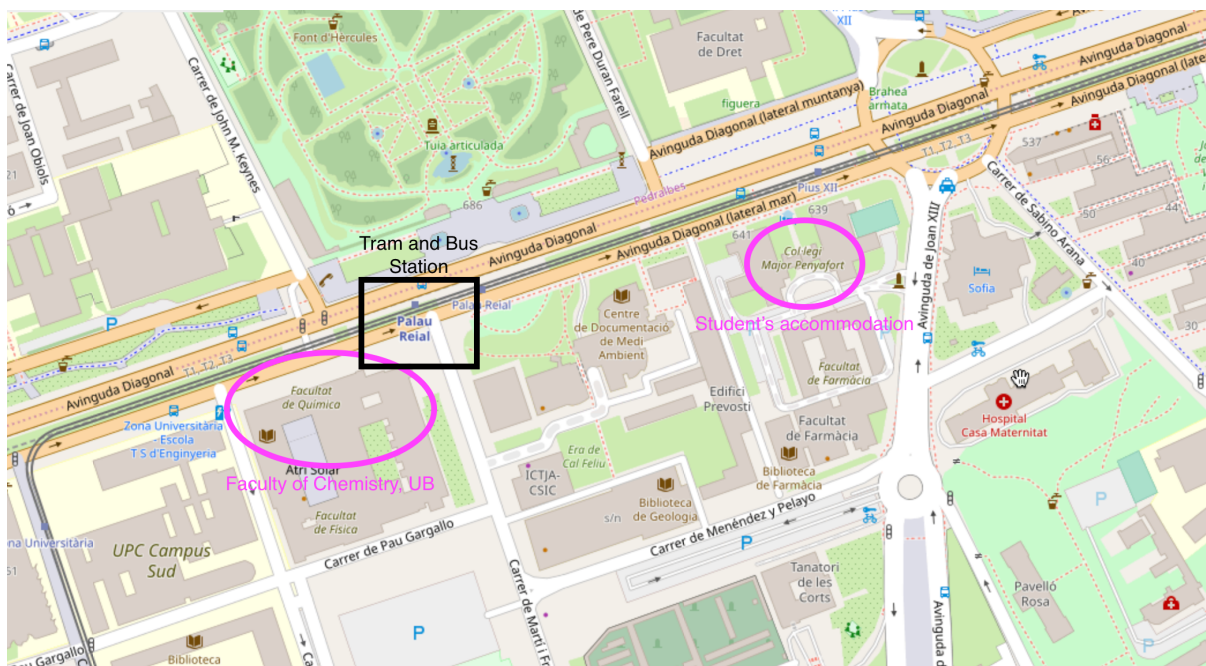
## Location

The workshop will be hosted by:

Facultat de Química Universitat de Barcelona  
(Faculty of Chemistry University of Barcelona)  
Carrer de Martí i Franquès 1, 08028 Barcelona

For a better orientation use [this map](#).





## Connecting to Wi-Fi

There are two ways of connecting to the iWi-Fi: First you can use your **eduroam** ID and use this URL to install it on your computer: <https://www.eduroam.org/eduroam-companion-app/> The second way to connect is using the Wi-Fi network of the University of Barcelona with the following settings:

WIFI name: wifi.ub.edu  
Identificador (USER NAME): bnfybm.tmp  
Contrasenya (PASSWORD): evuo56

## Accommodation

### Speakers and Tutors

All speakers and tutors are accommodated in the:

COL · LEGI MAJOR UNIVERSITARI SANT JORDI  
Paseig, Passatge de Ricard Zamora, 4, 8, 08017 Barcelona, Spain

For a better orientation use [this map](#).

To get to the University simply make a 25 minute walk or take the bus **H6** from *Mitre - Av Sarrià* to *Palau Reial* (during day time every 15 minutes)

## Participants

All participants are accommodated in the:

Col·legi Major Penyafort-Montserrat  
Avinguda Diagonal, 639-641, 08028 Barcelona, Spain

For a better orientation use [this map](#).

This accommodation is very close to the lecture halls and the computer rooms of Faculty of Chemistry. It is less than a 5-minute walk.

## Poster session

The suggested poster format is A0 in portrait orientation (1189mm high and 841mm wide). If absolutely necessary, poster printing is possible on site for a fee of roughly 15 EUR. Please contact Silvia Chellini ([schellini@ub.edu](mailto:schellini@ub.edu)).

## Poster Parade

In order to get to know each other, poster presenters will introduce themselves and their research in 90-second short presentation on the first day. For that, please upload a **\*\*SINGLE slide\*\*** in PDF format to [this online folder](#).

Please name your file **Last name\_First Name\_Registration-ID.pdf**

## Staying in touch

Share impressions of the workshop on twitter ([#DFTandBeyond19](#)).

To obtain daily updates on activities you can register at [Mattermost](#).

## Enjoying Barcelona

Eventhough it is the end of the summer it can still get hot in Barcelona. So, please don't forget your sunscreen and light clothes. There are also beaches around Barcelona. If you like to enjoy the Mediterranean Sea, you should not forget your swimming suite! How to get to the beach? The closest beach is the *La Barceloneta beach*. It takes about 40 minutes drive with public transport.

## 2 Program

<b>Monday August 26th Day 1: Data-driven materials discovery</b>		
12:00 - 14:30		Registration
14:30 - 14:45	The Organizers	Introductory remarks
14:45 - 15:45	Matthias Scheffler	Materials discovery from electronic-structure theory
15:45 - 16:45	Erich Runge	Density-functional theory
16:45 - 17:15	Coffee Break	
17:15 - 20:15		Poster parade and poster session

<b>Tuesday August 27th Day 2: Implementing DFT</b>		
09:00 - 10:00	Volker Blum	Practical implementations of DFT I: Technical foundations and numerical methods
10:00 - 11:00	Florian Knoop	Practical implementations of DFT II: SCF, forces, and structure optimization
11:00 - 11:30	Coffee Break	
11:30 - 12:30	Nicola Marzari	Plane-wave and pseudopotential methods
12:30 - 14:30	Lunch Break	
14:30 - 19:30		Tutorial 1: Basic aspects of using (high-performance) computing for materials modeling

<b>Wednesday August 28th Day 3: Accuracy and infrastructure</b>		
09:00 - 10:00	Sergey V. Levchenko	Periodic systems: Concepts and numeric atom-centered orbitals
10:00 - 11:00	Andreas Grüneis	Basics and state-of-the-art of quantum-chemistry methods for molecules, clusters, and materials
11:00 - 11:30	Coffee Break	
11:30 - 12:30	Alexandre Tkatchenko	Approaches to van der Waals interactions
12:30 - 14:30	Lunch Break	
14:30 - 19:30	Maria Dragoumi	Tutorial 2: The basics of electronic structure theory (molecules and clusters)

## 2 Program

<b>Thursday August 29th Day 4: Periodic systems, global search</b>		
09:00 - 10:00	Sergey V. Levchenko	Ab initio thermodynamics
10:00 - 11:00	Volker Blum	Electronic-Structure Infrastructure (ELSI)
11:00 - 11:30	Coffee Break	
11:30 - 12:30	Scott M. Woodley	Global optimization for nanosystems
12:30 - 14:30	Lunch Break	
14:30 - 15:30	David Casanova	The use of spin-flip excitations in DFT: theory and applications
15:30 - 19:30	Sara Jand	Tutorial 3: The basics of electronic structure theory (periodic systems)

<b>Friday August 30th Day 5: Thermodynamics and Time Evolution; Python-ASE</b>		
09:00 - 10:00	Weitao Yang	Recent developments in exchange-correlation functionals
10:00 - 11:00	Peter Kratzer	Kinetic Monte Carlo
11:00 - 11:30	Coffee Break	
11:30 - 12:30	Paul Kent	Quantum Monte Carlo
12:30 - 13:30	Morten Gjerding	Python-ASE and -ASR
13:30 - 15:30	Lunch Break	
15:30 - 19:30	Ask Hjorth Larsen	Tutorial 4: Python-ASE

<b>Saturday August 31th: Free Tutorials</b>		
		Excursion

<b>Sunday September 1st: Free Tutorials</b>		
17:00 - 20:00		Free Tutorials

<b>Monday September 2nd Day 6: Quasiparticle approaches: DFT and beyond</b>		
09:00 - 10:00	Patrick Rinke	Charged excitation (GW)
10:00 - 11:00	Claudia Draxl	Neutral Excitation (BSE)
11:00 - 11:30	Coffee Break	
11:30 - 12:30	Miguel Alexandre Marques	Neutral Excitations (TDDFT)
12:30 - 14:30	Lunch Break	
14:30 - 15:30	Xinguo Ren	RPA and Beyond
15:30 - 19:30	Dorothea Golze	Tutorial 5: Excited states and spectroscopy



## 2 Program

<b>Tuesday September 3rd Day 7: Transport and Reactions</b>		
09:00 - 10:00	Christian Carbogno	From Harmonic Vibrations to Strongly Anharmonic Heat Transport: Ab initio Nuclear Dynamics in Solids
10:00 - 11:00	Stefano Sanvito	Electronic transport – electron-spin coupling
11:00 - 11:30	Coffee Break	
11:30 - 12:30	Susan Sinnott	Reactive force fields for large simulations
12:30 - 14:30	Lunch Break	
14:30 - 15:30	Christian Carbogno	Electron-Phonon Coupling and Electronic Transport in Solids from First Principles
15:30 - 19:30	Florian Knoop	Tutorial 6: Phonons lattice, expansion, and band-gap renormalization

<b>Wednesday September 4th Day 8: Time and length scales</b>		
09:00 - 10:00	Karsten Reuter	Towards first-principles chemical engineering
10:00 - 11:30	Luca Ghiringhelli	Ab initio statistical mechanics and molecular dynamics
11:30 - 12:00	Coffee Break	
12:00 - 13:00	Danny Perez	Accelerated molecular dynamics
13:00 - 15:00	Lunch Break	
15:00 - 19:00	Yair Litman	Tutorial 7: Ab initio molecular dynamics

<b>Thursday September 5th Day 9: Multiscale and machine learning</b>		
09:00 - 10:00	Stefano Curtarolo	Entropy in materials modeling
10:00 - 10:30	Coffee Break	
10:30 - 11:30	Bjørk Hammer	Neural networks
11:30 - 12:30	Luca Ghiringhelli	Big-data analytics for materials science
12:30 - 14:30	Lunch Break	
14:30 - 19:30	Luca Ghiringhelli/Marcel Langer	Tutorial 8: Big-data analytics

## 2 Program

Friday September 6th Day 10: The Next Frontiers		
09:00 - 09:30	Claudia Draxl	The NOMAD project
09:30 - 10:00	Geoffroy Hautier	The Materials Project
10:00 - 10:30	Stefano Curtarolo	The AFLOW Project
10:30 - 11:00	Coffee Break	
11:00 - 11:45	Nicholas Hine	Electronic-structure theory for large-scale simulations
11:45 - 12:30	Nikolaj Moll	Quantum computing - Progress towards applications
12:30 - 12:45	The organizers	Closing remarks
12:45 - 13:45		Lunch and end of the School

# 3 Poster Abstracts

P1: - Surface engineering of lead hybrid perovskites for advanced photovoltaics . . . . .	13
P2: - Assessing Aqueous Stability of Nonequilibrium Nickel Chromium Oxides from First Principles . . . . .	14
P3: - Adsorption of porphyrin on metallic surfaces . . . . .	15
P4: - Methane Dehydrogenation on Transition Metal Nanoclusters: A Step-By-Step Quantum Chemistry Investigation . . . . .	15
P5: - High-throughput search for rare-earth-free permanent magnets . . . . .	16
P6: - First Principles Study: Elastic Properties of Cementitious Materials . . . . .	17
P7: - A DFT investigation of how polymer stabilising ligands affect nanoparticle catalysis	18
P8: - The manganese complex with redox non-innocent dioxolene ligands: computational study of the electronic and magnetic properties . . . . .	19
P9: - Electronic and Lattice Dynamical Properties of $MgTa_2O_6$ . . . . .	19
P10: - Theoretical investigation of magnons in Fe-Ga alloys . . . . .	20
P11: - Computational Electrochemistry of Water Oxidation on Metal - Doped and Metal - Supported Defective h - BN . . . . .	20
P12: - Modelling the CO <sub>2</sub> RR at the solid-liquid interface to understand the cation size effect . . . . .	21
P13: - Nature of Binding in Planar Halogen – Benzene Assemblies and Their Possible Visualization in Scanning Probe Microscopy . . . . .	22
P14: - On-surface synthesis of ethynylene bridged anthracene and pentacene polymers	23
P15: - Electric-Magneto-Optical Kerr Effect in a Hybrid Organic – Inorganic Perovskite	24
P16: - Electronic structure of perfect and imperfect cubic carbides . . . . .	24
P17: - Energetics and structure of Langmuir monolayers of palmitic acid: a DFT study	25
P18: - Scattering of Hydrogen Atoms at $\alpha$ -Al <sub>2</sub> O <sub>3</sub> Surfaces . . . . .	25
P19: - Morphological Changes in Nafion under Confinement and Protonation State/pH Variation . . . . .	26
P20: - Stability and Electronic Properties of the Palladium Dichalcogenides as Nanomaterials . . . . .	26
P21: - Analysis of peptide-chains and transport properties of polar amino-acids chains of different size. . . . .	27
P22: - Understanding Alloys and Metal Sulfides as Electrocatalysts for Nitrate Reduction	28
P23: - Benchmarking $G_0W_0$ calculations for open-shell molecules . . . . .	29
P24: - Investigation of the Elastic Properties of Binary Alloys through a mixed modelling-experimental approach . . . . .	29
P25: - Electronic Structure and Lithium Storage Mechanism of Niobium Oxide-based Crystallographic Shear Phases from First Principles . . . . .	30
P26: - MRChem for crystalline systems . . . . .	31
P27: - Time-resolved transport in quantum optoelectronic nanodevices . . . . .	31
P28: - Theoretical Design of Two-Dimensional Magnetoelectric materials . . . . .	32
P29: - Transport through nanostructures within the GW scheme . . . . .	32
P30: - Ab-initio quantum transport through atomic and molecular junctions . . . . .	33

P31: - A transferable machine-learning model for full-electron charge densities . . . . .	33
P32: - Predicting molecular conformers using Machine Learning . . . . .	34
P33: - Frustrated Structure Instability and Magnetism of superconducting $\text{KCr}_3\text{As}_3$ . . . . .	35
P34: - One Million Crystal Structures: One Million Disappearing Polymorphs Waiting to Happen? . . . . .	35
P35: - Modelling lithium intercalated graphite on the basis of semi-empirical electronic structure simulations with machine learning elements . . . . .	36
P36: - Computational Investigations of Ultrasmall Titanium Dioxide Nanoparticles . . . . .	37
P37: - Multiscale Modeling of Interface Effects on the Redox Chemistry of Ceria Nanoparticles . . . . .	37
P38: - A2P2, Python Package for Automated Atomistic Simulations . . . . .	38
P39: - Predicting magnetic dilution effects in mononuclear single molecule magnets . . . . .	39
P40: - Phonon symmetry selection in intralayer and interlayer electron-phonon interactions in twisted bilayer graphene . . . . .	39
P41: - DFT study of novel 3D C60 polymers . . . . .	40
P42: - Synergistic application of XPS and DFT to investigate Metal Oxide Surface Catalysis . . . . .	41
P43: - Ligand engineering in Cu(II) paddle wheel metal-organic frameworks for enhanced electrical conductivity . . . . .	42
P44: - Stabilizing Potential Superalloys . . . . .	42
P45: - Electronic and vibrational properties of Copper Indium Selenide: Impact of hybrid functionals on phonons . . . . .	43
P46: - Investigations of order-disorder phase transitions in high entropy alloys with the use of machine-learning interatomic potentials . . . . .	43
P47: - Graph similarity drives zeolite diffusionless transformations and intergrowth . . . . .	44
P48: - Phenylated Acene Derivatives as Candidates for Intermolecular Singlet Fission . . . . .	45
P49: - Tuning TCNQ adsorption on Ag(100): A joint DFT and experimental study of the role of alkali co-adsorption . . . . .	46
P50: - Reaction Mechanisms of the High Temperature Oxygen Evolution Reaction . . . . .	46
P51: - DFT based screening for oxide supported catalyst materials . . . . .	47
P52: - All-Zinc Coordinated Nickel-Complexes as Molecular Mimics for NiZn Catalyst Surfaces, a Density Functional Theory Study . . . . .	48
P53: - <b>The Role of Charge Transfer in the <math>\text{CO}_2</math> Activation on <math>3d</math> <math>\text{TM}_{13}</math> Clusters: A DFT Investigation</b> . . . . .	48
P54: - <i>Ab initio</i> Investigation of Mixture of $\text{CeO}_2$ - $\text{ZrO}_2$ Nanoclusters and Adsorption of Zr-adatoms on the $\text{CeO}_2$ (111) Surface . . . . .	49
P55: - Bandgap and pseudohelicity effects over conductance in gapped graphene junctions . . . . .	50
P56: - The dynamic structure factor of warm dense copper . . . . .	50
P57: - <i>Ab initio</i> molecular dynamics simulations of negative thermal expansion in $\text{ScF}_3$ : the effect of the supercell size . . . . .	51
P58: - Experimental and theoretical study of nanoshaped Ni/ $\text{CeO}_2$ catalysts for hydrogen production . . . . .	52
P59: - Exact-exchange effects in hybrid exchange-correlation functionals to describe metal oxides . . . . .	53
P60: - Sites for CO dissociation over platinum . . . . .	54
P61: - $\text{CO}_2$ methanation reaction on the Ni(111) surface: first-principles kinetic Monte Carlo study . . . . .	54
P62: - Unraveling Morphological and Topological Key Aspects of Pd Nanoparticles . . . . .	55

### 3 Poster Abstracts

P63: - Subsurface Carbon: A General Feature of Noble Metals . . . . .	56
P64: - Morphology Dependence of Stability and Properties of Stoichiometric TiO <sub>2</sub> Nanoparticles . . . . .	57
P65: - Entanglements and Information Theoretic Measures in Nanostructure Systems .	57
P66: - Thermal Transport in Si/Ge Nano-Grains using Ab-initio Simulations . . . . .	58
P67: - <i>In silico</i> characterisation of anharmonic free energies of molecular crystals . . .	59
P68: - Electrochemical doping of HfNCl: spin-orbit coupling, spin texture, and Ising superconductivity . . . . .	60
P69: - Second-order Møller-Plesset perturbation theory and beyond for the band gap and single-particle excitations of solids . . . . .	60
P70: - Representations of molecules and materials for interpolation of ab initio calculations	61
P71: - Interplay of quantum nuclear fluctuations and the electronic structure of the cyclohexane/Rh(111) interface . . . . .	62
P72: - Interplay of quantum nuclear fluctuations and the electronic structure of the cyclohexane/Rh(111) interface . . . . .	62
P73: - Fully-Anharmonic, First-Principles Theory of Electronic Transport . . . . .	63
P74: - Blueprint strategy for cation-peptide force-field parameterization . . . . .	63
P75: - Accelerating the High-Throughput Search for Strongly Anharmonic Thermal Insulators . . . . .	64









---

## Surface engineering of lead hybrid perovskites for advanced photovoltaics

P1

Aleksandra Oranskaia\* and Udo Schwingenschlöggl\*

\* *King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC), Thuwal 23955-6900, Saudi Arabia*

Despite enormous progress in material characterization, there is still a great lack of knowledge about the atomic scale surface reconstructions in photovoltaic devices. This is particularly critical, because the majority of charge carrier losses occurs at surfaces and interfaces [1,2]. In addition, surfaces and interfaces are starting points of material deterioration. We employ first-principles modeling based on density functional theory to overcome this knowledge gap, focusing on perovskite absorber materials used in new generation solar cells [3]. We aim at establishing structure-property relationships that can lead to strategies for improving the power conversion efficiency of lead hybrid perovskite solar cells by elucidating their surface reconstructions and the related electronic properties. The investigation is executed in the context of evolutionary crystallography as implemented in the USPEX package [4-6] in combination with Quantum Espresso [7].

- [1] X. Wu et al., Trap states in lead iodide perovskites, *J. Am. Chem. Soc.* 137, 2015, pages 2089-2096
- [2] W. Kong et al., Optical characterizations of the surface states in hybrid lead-halide perovskites, *Phys. Chem. Chem. Phys.* 18, 2016, pages 12626-12632
- [3] N.-G. Park et al., Organic-inorganic halide perovskite photovoltaics. *From Fundamentals to Device Architectures* (Springer, Berlin, 2016)
- [4] A. R. Oganov and C.W. Glass. Crystal structure prediction using ab initio evolutionary techniques: Principles and applications, *J. Chem. Phys.* 124, 2006, article 244704
- [5] A. O. Lyakhov et al., New developments in evolutionary structure prediction algorithm USPEX, *Comp. Phys. Comm.* 184, 2013, pages 1172-1182
- [6] A. R. Oganov et al., How evolutionary crystal structure prediction works - and why, *Acc. Chem. Res.* 44, 2011, pages 227-237
- [7] P. Giannozzi et al., QUANTUM ESPRESSO: A modular and open-source software project for quantum simulations of materials, *J. Phys.: Condens. Matter* 21, 2009, article 395502

---

## Assessing Aqueous Stability of Nonequilibrium Nickel Chromium Oxides from First Principles

P2

Kathleen Mullin\* and James Rondinelli\*

\* *Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208, USA*

Ni-Cr alloys are used in high temperature applications, such as resistance heating elements, where corrosion resistance is critical to performance. It has generally been thought that this corrosion resistance comes from a passive film made of NiO with the rock salt crystal structure, Cr<sub>2</sub>O<sub>3</sub> with the corundum crystal structure, or a Ni-Cr oxide with the spinel crystal structure forming on the metals surface. Recently, however, new data shows that valence-precise compositions and bulk equilibrium structures do not necessarily form in the ultrathin limit, raising questions about the suitability of existing bulk thermodynamic models. Specifically, in aqueous environments, Ni-Cr alloys form nonequilibrium phases through a solute capture process, whereby Ni-Cr oxide in the rock salt structure with unexpectedly large solubility of Cr on the Ni lattice occurs [1]. In order to better understand the formation of this nonequilibrium oxide, we use ab-initio Density Function Theory (DFT) calculations to parameterize a cluster expansion model of the Ni-Cr-O system in the rock salt structure as a function of Cr content. We seek to assess the important simple and multi-body interactions that govern stability of the non-equilibrium oxides. Next, we use energies of formation derived from the cluster-expansion to create electrochemical Pourbaix diagrams to better understand the stability of the oxide in over a range of pH and potential values.

- [1] Xiao-xiang Yu, Ahmet Gulec, Quentin Sherman, Katie Lutton Cwalina, John R. Scully, John H. Perepezko, Peter W. Voorhees, and Laurence D. Marks, Nonequilibrium solute capture in passivating oxide films, *Phys. Rev. Lett.* 121 (2018), 145701.

---

## Adsorption of porphyrin on metallic surfaces

P3

Shabnam Naseri\*

\* (*PhD candidate*) *Applied Physics, Division of Materials Science, Department of Engineering Sciences and Mathematics, Luleå University of Technology, Sweden.*

In recent years the investigation of porphyrin molecules on surfaces is of great interest because of their potential applications in several fields like photonics [1], molecular electronics [1] and solar cells [2]. Their impressive variety of functional properties and the fact that they are extraordinarily stable makes them perfect candidates in these fields. Since one research part of the porphyrins is focused on their use as elements for future molecular electronic systems, the interaction between them and surfaces is very important. We study in detail the interaction of porphyrin molecules with the Cu(111) and Ag(111) surfaces by means of density functional theory calculations (DFT). More specific, we study the electronic and geometric differences of the adsorbed porphyrins in order to see the type of interactions (chemical interaction, attractive van der Waals interactions) between the molecule and different surfaces. A detailed study of different molecule - surface interactions is essential for a comprehensive analysis and interpretation of experimental data since conformational changes due to the adsorption of the molecule can affect its properties and the mechanisms that drive these changes are often unclear.

- [1] Jurow et al., *Coordination chemistry reviews*, 2010, 2297  
 [2] Tountas et al., *ACS Applied Materials and Interfaces*, 2018, 20728

## Methane Dehydrogenation on Transition Metal Nanoclusters: A Step-By-Step Quantum Chemistry Investigation

P4

Karla F. Andriani\* and Juarez L. F. Da Silva\*

\* *São Carlos Institute of Chemistry, University of São Paulo, São Carlos, São Paulo, Brazil*

The conversion of methane ( $\text{CH}_4$ ) into new products such as methanol can provide a new route for a transitional energy sustainability world due the large supply of methane world wide, in particular, Brazil, however, there are great challenges to achieve this goal in special at low temperature due to the high stability of the C–H bonds.[1],[2] Therefore, there is a great interest to design new catalysts for the  $\text{CH}_4$  conversion, which can be based on distinct materials.[3],[4] At this work, we will explore transition-metal particles to study step-by-step the reaction conversion of  $\text{CH}_4$  into methanol under full-lean oxygen conditions. For that, we have employed computational quantum chemistry based on *ab initio* DFT calculations to shed light on the first step of the reaction mechanism regarding the methane dehydrogenation on transition metal nanoclusters ( $\text{M}_{13}$  with  $\text{M} = \text{Fe}, \text{Co}, \text{Ni}, \text{and Cu}$ ). The cluster adsorption algorithm was used to achieve an accurate description of each adsorbed system  $\text{M}_{13}\text{X} + \text{CH}_{4-X}$  ( $\text{X}=1-4$ ) through the generation of approximately 10 million trial configurations that were later refined into a representative set of 20-30 configurations using the Euclidean similarity distance algorithm (ESD). We found that the adsorption of methane and the dehydrogenation species i.e.  $\text{CH}_3$ ,  $\text{CH}_2$ ,  $\text{CH}$ , and  $\text{C}$ , on  $\text{M}_{13}$  nanoclusters is guided by the change on the  $\text{sp}^3$  carbon hybridization which leads to distinct coordination bonding preferences. For instance, we observed that the 4-coordinated bonding is achieved for only  $\text{Fe}_{13}+\text{C}$  system, while in  $\text{Cu}_{13}$  nanoclusters the same pattern occurs for  $\text{C}$  and  $\text{CH}$  systems. In addition, our results suggest a tendency of  $\text{Fe}_{13}+\text{CH}$  to rearrange as  $\text{Fe}_{13}+\text{C}$  systems, which highlight the iron catalysts tendency to form carbon depositions. Regarding the stability, the  $\text{CH}_3$  specie when adsorbed on both  $\text{Fe}_{13}$  and  $\text{Cu}_{13}$  nanoclusters yield the most stable systems, and as expected the adsorption of  $\text{CH}_4$  is energetically unfavorable in reason of its physisorption nature. However, in general, the dehydrogenation species have a stronger interaction with  $\text{Fe}_{13}$  nanocluster except for methane as a consequence of the higher adsorption energy magnitude ( $E_{ad} = -0.6$  eV) for  $\text{Cu}_{13}$  in comparison with  $\text{Fe}_{13}$  ( $E_{ad} = -0.2$  eV) nanocluster.

[1] Arevalo, R. L. et al. Sci. Rep. 2017, 7, 13963, 1-7.

[2] He, J. et al. Fuel 2018, 226, 400-409.

[3] Chaves, A. S. et al. Phys. Chem. Chem. Phys. 2017, 19, 15484-15502.

[4] Chaves, A. S. et al. J. Phys. Chem. A 2015, 119 (47), 11565-11573.

## High-throughput search for rare-earth-free permanent magnets

P5

Alena Vishina\*, Olga Yu. Vekilova\*, Olle Eriksson\*,† and Heike C. Herper\*

\* *Uppsala University, Uppsala, Sweden*

† *School of Science and Technology, Orebro University, SE-701 82 Orebro, Sweden*

High performance permanent magnets, or materials with large uniaxial magnetic anisotropy, are needed for a large number of applications, such as electric motors and generators, wind mills, and many more. At the same time these days most high performance magnets contain rare-earth (RE) materials which makes them expensive, while some of the RE elements (like Dy) are rapidly decreasing in availability. According to the assessment of European Union in 2014 not only the RE elements, but also Pt and Co, and phase stabilizers like Ge and In, used in permanent magnets, have been classified as critical raw materials.

Going through a large number of known structures (ICSD database [1]) and using a full-potential linear muffin-tin method with relativistic formulation in RSPt electron structure code [2] to calculate magnetic anisotropy and Curie temperature, we are looking for the materials with high magnetization  $> 1$  T, uniaxial anisotropy  $> 1$  MJ/m<sup>3</sup>, and  $T_c > 300$  K to identify the suitable replacement for hazardous materials, without a loss of performance in permanent magnets.

Authors would like to acknowledge the support of the Swedish Foundation for Strategic Research and Swedish National Infrastructure for Computing (SNIC) for the computation resources.

[1] [www2.fiz-karlsruhe.de](http://www2.fiz-karlsruhe.de)

[2] John M. Wills et al., arXiv:cond-mat/9912173 (1999)

---

## First Principles Study: Elastic Properties of Cementitious Materials

P6

J. S. Rego\*, S. M. Mutisya<sup>‡</sup>, C. R. Miranda<sup>†</sup> and M. de Koning\*

\* *Gleb Wataghin Institute of Physics, University of Campinas, Campinas-SP, 13083-859, Brazil*

<sup>†</sup> *Institute of Physics, University of São Paulo, São Paulo-SP, 05508-090, Brazil*

<sup>‡</sup> *SUBATECH, UMR CNRS 6457, IN2P3/IMT Atlantique/Université de Nantes, 44307, Nantes, France*

Concrete is the most used material in the civil construction industry and has long attracted countless researches, mainly on its physico-chemical properties, also on its atomic structure and microstructure, which are still not completely understood and solved, as well as the improvement of its performance. Concrete is composed basically of cement, water and aggregates, and its resistance and contraction properties are related to the hydrated phase of the cements. In the usual Portland cement we have the Calcium Silicate Hydrate, abbreviated as CSH ( $(\text{CaO})_x\text{-SiO}_2\text{-(H}_2\text{O)}_y$ ) and the new magnesium based cements have the Magnesium Silicate Hydrate, abbreviated as MSH ( $(\text{MgO})_x\text{-SiO}_2\text{-(H}_2\text{O)}_y$ )[1,2]. Both are almost amorphous materials with their structures not yet well determined. Studies in the literature have shown that CSH exhibits sharp peaks in WAXS (Wide Angle X-Ray Scattering) patterns characteristic of the mineral tobermorite, whose chemical formula is  $\text{Ca}_5(\text{Si}_6\text{O}_{16}(\text{OH})_2)\cdot 4(\text{H}_2\text{O})$ , while that M-S-H shows some broad and poorly defined peaks, typical of an amorphous phase, which can be attributed to those of the lizardite  $(\text{Mg,Fe})_3(\text{Si}_2\text{O}_5)(\text{OH})_4$  and that of talc,  $\text{Mg}_6(\text{Si}_8\text{O}_{20})(\text{OH})_4$ [3-5]. To understand and predict the behavior of these materials it is necessary to determinate their structures. Atomistic simulations are a great tool for this purpose, allowing the study of the properties and structure of these materials on nano and microscales. In this work we study the electronic structure of these mineral linked to the cementitious phases CSH and MSH, using ab initio calculations. Specifically, we employ Density Functional Theory (DFT)

using the plane-wave basis projector augmented wave method and generalized gradient approximation in the Perdew- Burke-Ernzenhof (PBE) as implemented in VASP package. From the first principles calculations we obtained the structural parameters and the elastic properties in the linear regime of these minerals, we observed the influence of possible impurities of magnesium and the amount of water in the chemical structure of the Tobermorite and carried out a comparative study of its elastic properties, such as Young modulus, Shear modulus, Bulk modulus and Poisson Ratio with those of magnesium silicates Talc and Lizardite. Experimental studies indicate that MSH has poorer mechanical properties compared to CSH. In this comparative study, we can indicate through the elastic properties of these materials which of the hydrated phases are more mechanically stable and which structures are closer to the experimentally observed.

- [1] I. Jawed, J. Skalny, J.F Young., *Struct. Perform. Cem.* (1983), 284-285.
- [2] B. Lothenbach et al., *Cement and Concrete Research* 77 (2015) 60 – 68.
- [3] Chiang, W.S. et al., *J. Mater. Chem. A* 2014, 2 (32), 12991 – 12998.
- [4] He, Y. H. et al., *Wuhan Univ. Technol.Mater. Sci. Ed.* 2011, 26 (4), 770 – 773.
- [5] Mellini, M. et al., *Mineral. Mag.* 2010, 74 (2), 277 – 284.

---

## A DFT investigation of how polymer stabilising ligands affect nanoparticle catalysis

P7

Mahmoud Mansi\* and Andrew Logsdail\*  
\* *Cardiff Catalysis Institute, Cardiff University*

In chemistry, catalysts facilitate a reaction without being consumed themselves. Catalysis, which is any chemical process involving a catalyst, underpins modern society, contributing in the synthesis of almost all (>90

Currently, understanding how a catalyst works, and then designing improvements, is hampered by the lack of detailed characterisation that is feasible during reactions. A simple example of this is the role of stabilising polymer ligands that are typically used to encapsulate metal nanoparticle catalysts. [1] What does the ligand do? How does it interact with the nanoparticles? And is involved in the catalytic reaction itself? Answering these difficult questions will be of fundamental in the growing application of these systems, and therefore further research is needed.

Whilst knowledge of how catalysts work is limited, the advent of modern computing technologies provides a pathway to mechanistic information through atomic simulations, which can make accurate experimental predictions. Such computational approaches are to be harnessed in my work, where , I will be investigating how polymer ligands impact surface chemistry. In particular, I will be using the software package “FHI-aims” to perform ab initio simulations of these systems[2]. My research is currently in the very early stages, having only commenced in April 2019, but I hope to present some insight into these challenges, and outline the next work I will be pursuing, through this Poster presentation.

- [1] Robert B. Grubbs (2007) Roles of Polymer Ligands in Nanoparticle Stabilization, *Polymer Reviews*, 47:2, 197-215, DOI: 10.1080/15583720701271245
- [2] V. Blum et al (2009) Ab initio molecular simulations with numeric atom-centered orbital, *Computer Physics Communications* Volume 180, Issue 11, November 2009, Pages 2175-2196.

## The manganese complex with redox non-innocent dioxolene ligands: computational study of the electronic and magnetic properties

E. M. Kadilenko<sup>\*,†</sup>, A. A. Dmitriev<sup>\*,†</sup> and N. P. Gritsan<sup>\*,†</sup>

<sup>\*</sup> *Novosibirsk State University, Russia, 630090, Novosibirsk, 1 Pirogora str.*

<sup>†</sup> *Institute of Chemical Kinetics and Combustion, Russia, 630090, Novosibirsk, 3 Institutskaya str.*

Transition metal complexes with redox non-innocent ligands are among the most interesting objects of modern coordination chemistry. The most popular redox non-innocent ligands are the dioxolene type ligands derived from o-quinones (Q), which can be in the dianionic catecholate (Cat), o-semiquinone (SQ) or neutral (Q) forms. Such complexes are very challenging for computational quantum chemistry due to their nontrivial open-shell nature. Thus, only *ab initio* multi-configurational methods are appropriate to correctly predict their unusual electronic structure.

In recent study [1], a new tris-dioxolene manganese complex ( $Mn(Diox)_3$ , **1**) was synthesized and characterized using X-ray diffraction and magnetic susceptibility measurements (Diox is derived from the 3,6-di-tert-butyl-o-benzoquinone having a N,N'-piperazine bicycle as substituent in 4,5-positions, DBQ-pipe). The localized oxidation state of **1**,  $Mn^{IV}(Cat)(DBSQ - pipe)_2$ , was proposed by the authors. We estimated the empirical metric oxidation states (MOS) of the ligands using the XRD structure and recently proposed procedure [2]; the estimations led to the MOS values being -1.00, -1.42 and -1.35, which does not agree with proposed oxidation states. The goal of our study was to reveal the electronic structure and properties of **1** using multi-configuration *ab initio* approach.

Calculations were performed at the SA-CASSCF(7,8)/NEVPT2 level with active space consisting of 7 electrons and 8 orbitals, which are five 3d-orbitals and 3 LUMOs of the ligands. A series of calculations were done with different numbers of the accounted electronic states with  $S = 1 \quad 2 \div 7 \quad 2$ . The ground ( $E_1 = 0$ ) and first excited ( $E_2 \approx 350cm^{-1}$ ) states were predicted to be doublets with the third state being quartet ( $E_3 \approx 890cm^{-1}$ ). Calculations predict a number of lowest-energy states of **1** with wavefunctions characterized by the occupation of 7 active orbitals by 1 electron and one unoccupied d-orbital. Thus, all these states arise from the antiferromagnetic interaction between  $Mn^{III}$  (with  $S = 2$ ) and three DBSQ-pipe radical anions ( $S = 1 \quad 2$ ). Therefore, the electronic structure of complex **1** can be described as  $Mn^{III}(DBSQ - pipe)_3$ . Analysis of all computational results will be presented and discussed. This work was supported by the Russian Foundation for Basic Research (project 18-33-00143).

[1] Bubnov, M. et al. (2019). *Inorganica Chimica Acta*, 486, 113-118.

[2] Brown, S. N. (2012). *Inorganic chemistry*, 51(3), 1251-1260.

---

**Electronic and Lattice Dynamical Properties of  $\text{MgTa}_2\text{O}_6$** 

P9

Kyle D. Miller\* and James M. Rondinelli\*

\* *Northwestern University*

Materials exhibiting metal-insulator transitions (MIT) are proposed platforms for next-generation low-power electronics. In addition, most of these materials exhibit strong coupling between the electronic and lattice degrees-of-freedom, which makes them ideal systems to examine the interplay between lattice dynamics, electronic structure, and magnetic order. Well-studied rutile-structured MIT oxides, such as  $\text{VO}_2$  and  $\text{NbO}_2$ , exhibit dimerized cations within the edge-connected octahedra along the  $c$  axis in the insulating state [1,2]. Analogous compounds with the related trirutile superstructure, e.g.,  $\text{V}_2\text{WO}_6$  [1] and  $\text{CuSb}_2\text{O}_6$  [3], exhibit a similar dimerization. Here we investigate the MIT behavior in  $\text{MgTa}_2\text{O}_6$ , a  $d^0$  insulator with the potential to be electron doped into a metallic state susceptible to a Peierls-type MIT. Our calculations suggest that  $\text{MgTa}_2\text{O}_6$  remains metallic for electron doping configurations within the  $d^{0.25}$ - $d^{0.5}$  range, whereas a dimerization occurs for much higher values. Overall, these results indicate that trirutile oxides may be a promising materials class for which to functionalize MITs.

- [1] Hiroi, Z. Structural instability of the rutile compounds and its relevance to the metal-insulator transition of  $\text{VO}_2$ . *Prog. Solid State Ch.* 43, 47-69, 2015; 10.1016/j.prog-solidstchem.2015.02.001
- [2] O' Hara A and Demkov A. Nature of the metal-insulator transition in  $\text{NbO}_2$ . *Phys. Rev. B*, 91, 094305, 2015; 10.1103/PhysRevB.91.094305
- [3] Golubev A, Dinnebier R, Schulz A, and Kremer RK. Structural and Magnetic Properties of the Trirutile-type 1D-Heisenberg Anti-Ferromagnet  $\text{CuTa}_2\text{O}_6$ . *Inorg. Chem.* 56, 6318-6329, 2017; 10.1021/acs.inorgchem.7b00421

---

**Theoretical investigation of magnons in Fe-Ga alloys**

P10

Gustav Johansson\*, Oleg Gorbatov\* and Corina Etz\*

\* *Luleå University of Technology*

Dilute solid-solution magnetostrictive Fe-alloys are of great interest with potential applications in sensors and transducers. Fe-Ga alloys of certain concentrations show an unusually large increase in magnetostriction compared to pure Fe. For this reason they are the most interesting Fe-based alloys. In this study, we describe the magnetic interactions in Fe-Ga alloys by means of ab initio fully-relativistic electronic structure calculations. Moreover, we investigate the Curie temperatures, spin-wave excitations spectra and spin-wave stiffness as a function of Ga-concentration. The effect of disorder, as reflected in the magnon spectra, is investigated in detail. The spectra have been modeled using atomistic spin dynamics simulations. The possibility of high throughput calculations for other Fe-based alloys with different concentrations is also discussed.

- [1]

---

## Computational Electrochemistry of Water Oxidation on Metal-Doped and Metal-Supported Defective h-BN

P11

Daniele Perilli\*, Daniele Selli\*, Hongsheng Liu\* and Cristiana Di Valentin\*

\* *Dipartimento di Scienza dei Materiali, Università di Milano Bicocca, via R. Cozzi 55, 20125 Milano (Italy)*

Metal-doped and metal-supported two-dimensional materials are attracting a lot of interest as potentially active electrocatalysts for reduction and oxidation processes [1,2,3]. Previously, when a non-regular 2D h-BN layer was grown on a Cu(111) surface, metal adatoms were found to spontaneously emerge from the bulk to fill the atomic holes in the structure and become available for surface catalysis [4]. Herein, computational electrochemistry is used to investigate and compare the performance of Cu-doped and Cu-supported pristine and defective h-BN systems for the electrocatalytic water oxidation reaction. For the various model systems, the intermediate species of this multistep oxidation process are identified and the free-energy variations for each step of reaction are computed, even for those steps that do not involve an electron or a proton transfer. Both associative and O<sub>2</sub> direct evolution mechanisms are considered. On this thermodynamic basis, the potential-determining step, the thermodynamic-determining step, and consequently the theoretical overpotential are determined for comparison with experiments. Small Cu clusters (tetramers) trapped in the h-BN defective lattice on a Cu(111) support are found to be very active for the water oxidation reaction since such systems are characterized by a low overpotential and by a small energy cost for O<sub>2</sub> release from the catalyst, which is often observed to be a major limit for other potential electrocatalysts [5].

- [1] K. Uosaki, G. Elumalai, H. Noguchi, T. Masuda, A. Lyalin, A. Nakayama, T. Taketsugu, *J. Am. Chem. Soc.*, 136, 6542 – 6545, (2014).
- [2] J. Zhao, Z. Chen, *J. Am. Chem. Soc.*, 139, 12480 – 12487, (2017).
- [3] G. Hu, Z. Wu, S. Dai, D. Jiang, *ACS Appl. Mater. Interfaces*, 10, 6694 – 6700, (2018).
- [4] D. Perilli, D. Selli, H. Liu, E. Bianchetti, C. Di Valentin, *J. Phys. Chem. C*, 122, 23610-23622, (2018).
- [5] D.Perilli, D. Selli, H. Liu, C. Di Valentin, *ChemSusChem*, asap, DOI: 10.1002/cssc.201802499 (2019)

---

## Modelling the CO<sub>2</sub>RR at the solid-liquid interface to understand the cation size effect

P12

Pulumati Sri Harsha\*, Ebrahim Tayyebi\* and Egill Skúlason\*

\* *University of Iceland*

The dream for a sustainable future is to be able to capture CO<sub>2</sub> gas from both industrial sources and the atmosphere and convert it to hydrocarbons and alcohols, which can be used as synthetic fuels or other carbon products. An appealing approach is to use CO<sub>2</sub> as a reactant and a renewable



energy source to make synthetic fuels or plastics. The problem with electrochemical CO<sub>2</sub> reduction reaction (CO<sub>2</sub>RR) is that, energy-efficient and selective catalyst has not yet been identified. Cu is the only pure metal electrode tested so far that generates any significant yield, whereas other pure metal electrodes make only H<sub>2</sub>, CO or formate [1].

Recently, it has been found that CO<sub>2</sub>RR can be influenced by an alkali metal cation in the electrolyte, where its size can affect selectivity and activity of CO<sub>2</sub>RR significantly. However, the reason for that has not been understood fully yet on a molecular level. The theoretical work done so far in order to gain insight into these effects suffer from a limited number of explicit water molecules [2] or that an ice like bilayer of water is used [3]. In this work, we are using ab initio molecular dynamics simulations with a higher number of explicit water molecules on a Cu(111) electrode to get a better understanding of the effect of cation size and its solvation with water molecules. The aim of this work is to build a better model for the interface between Cu(111) and water with various cations (e.g. Li, Na, K, Cs) in order to calculate the product distribution for CO<sub>2</sub>RR when different cations are used, and compare that with the experiments [4,5].

- [1] D. T. Whipple and P. J. Kenis, "Prospects of CO<sub>2</sub> utilization via direct heterogeneous electrochemical reduction," ACS Publications, vol. 1, no. 24, pp. 3451–3458, 2010.
- [2] J. Resasco, L. D. Chen, E. Clark, C. Tsai, C. Hahn, T. F. Jaramillo, K. Chan and A. T. Bell, "Promoter effects of alkali metal cations on the electrochemical reduction of carbon dioxide," Journal of the American Chemical Society, vol.139, no. 32, pp. 11277–11287, 2017.
- [3] J. Mills, I. McCrum and M. Janik, "Alkali cation specific adsorption onto fcc(111) transition metal electrodes," Physical Chemistry Chemical Physics, vol.16, no. 27, pp. 13699–13707, 2014.
- [4] M. R. Singh, Y. Kwon, Y. Lum, J. W. Ager III and A. T. Bell, "Hydrolysis of electrolyte cations enhances the electrochemical reduction of CO<sub>2</sub> over Ag and Cu," Journal of the American Chemical Society, vol. 138, no. 39, pp. 13006-3012, 2016.
- [5] J. Hussain, H. Jónsson and E. Skúlason, "Calculations of product selectivity in electrochemical CO<sub>2</sub> reduction," ACS Catalysis, vol. 8, no. 6, pp. 5240-249,2018.

---

## Nature of Binding in Planar Halogen – Benzene Assemblies and Their Possible Visualization in Scanning Probe Microscopy

P13

Aurelio Gallardo<sup>\*,†</sup>, Jindrich Fanfrlík<sup>‡</sup>, Pavel Hobza<sup>‡,4</sup> and Pavel Jelínek<sup>\*,4</sup>

<sup>\*</sup> *Institute of Physics of the Czech Academy of Sciences, 162 00 Prague, Czech Republic*

<sup>†</sup> *Faculty of Mathematics and Physics, Charles University, 180 00 Prague, Czech Republic*

<sup>‡</sup> *Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, 166 10 Prague, Czech Republic*

<sup>4</sup> *Regional Centre of Advanced Technologies and Materials, Palacký University, 78371 Olomouc, Czech Republic*

High-resolution scanning probe imaging of molecular structures on surfaces with functionalized tips provided the unprecedented spatial resolution. However, the origin of sharp intermolecular features often presented in high-resolution images of molecular assemblies is still under intensive debate.

Originally, such features were considered as a direct observation of weak non-covalent bonds between molecules. Nevertheless, this interpretation was challenged and ascribed to an experimental artefact. To address this long-standing controversy, we provided theoretical analysis of intermolecular interaction and high-resolution imaging of halogen substituted benzenes assemblies deposited on metallic substrate, which was extensively studied experimentally.[1] First, we show that formation of molecular assemblies made of  $C_6Br_6$  and  $C_6F_6$  on surfaces is driven by interplay between halogen and dispersive interaction. Next, for the  $C_6Br_6$  and  $C_6F_6$  assemblies on surface we analyze simulated high-resolution inelastic electron tunneling spectroscopy (IETS) and atomic force microscopy (AFM) images acquired with a CO-tip.[2],[3] Very good agreement with the experimental evidence allows us to unambiguously determine that the lateral bending of CO-tip due to Pauli repulsion is responsible for the intermolecular sharp edges. In addition, we discuss, why such sharp features should not be interpreted as the direct evidence of the signature of weak non-covalent bonds.

- [1] Z. Han et al., *Science* 358, 206-210 (2017)
- [2] P. Hapala et al., *Phys. Rev. Lett.* 113, 226101 (2014)
- [3] P. Hapala, *Phys. Rev. B* 90, 085421 (2014)
- [4] P. Jelinek, *J. Phys.: Condens. Matter* 29, 343002 (2017)
- [5] M. H. Kolár et al., *Chem. Rev.* 116, 5155-5158 (2016)
- [6] A. Gallardo et al., *J. Phys. Chem. C*, (2018)

---

## On-surface synthesis of ethynylene bridged anthracene and pentacene polymers

P14

Shayan Edalatmanesh\*, Ana Sánchez-Grande<sup>†</sup>, Bruno de la Torre<sup>\*,‡</sup>, José Santos<sup>†</sup>, Borja Cirera<sup>†</sup>, Koen Lauwaet<sup>†</sup>, Taras Chutora\*, Pingo Mutombo<sup>‡</sup>, Johanna Rosen<sup>4</sup>, Radek Zbořil\*, Rodolfo Miranda<sup>†</sup>, Jonas Björk<sup>4</sup>, Pavel Jelínek<sup>\*,‡</sup>, Nazario Martín<sup>†,5</sup> and David Écija<sup>†</sup>

\* *Regional Centre of Advanced Technologies and Materials, Palacký University*

† *IMDEA Nanociencia*

‡ *Institute of Physics, The Czech Academy of Sciences*

<sup>4</sup> *Department of Physics, Chemistry and Biology, IFM Linköping University*

<sup>5</sup> *Departamento de Química Orgánica, Facultad de Ciencias Químicas, Universidad Complutense*

Engineering low bandgap pi-conjugated polymers is a burgeoning area in basic and applied research, with the main synthetic challenge being in the solubility of the materials during the chemical synthesis. Here we report a comprehensive study of the on-surface synthesis of anthracene and pentacene based, low-bandgap molecular wires on Au(111) using scanning tunneling microscopy (STM), non-contact atomic force microscopy (nc-AFM), density functional theory (DFT) and complementary AFM/STM simulations [1]. Our results not only introduce a ground-breaking chemical protocol to design pi-conjugated polymers based on oligoacene precursors, but also shed light upon the aromatic-quinoid transition in named systems and the transformation of ethynylene bridge bonds between polyacene moieties. Thus contributing to the development of the field of on-surface chemistry and the design of modern low bandgap polymers.

- [1] Sánchez - Grande, A. , de la Torre, B. , Santos, J. , Cirera, B. , Lauwaet, K. , Chutora, T. , Edalatmanesh, S. , Mutombo, P. , Rosen, J. , Zbořil, R. , Miranda,

R. , Björk, J. , Jelínek, P. , Martín, N. and Écija, D. (2019), On - Surface Synthesis of Ethynylene - Bridged Anthracene Polymers. *Angew. Chem. Int. Ed.* doi:10.1002/anie.201814154

---

## Electric-Magneto-Optical Kerr Effect in a Hybrid Organic-Inorganic Perovskite

P15

Feng-Ren Fan\*, Hua Wu\*,<sup>†</sup>, Dmitrii Nabok<sup>‡</sup>, Shunbo Hu<sup>4</sup>, Wei Ren<sup>4</sup>, Claudia Draxl<sup>‡</sup> and Alessandro Stroppa<sup>5</sup>

\* *Laboratory for Computational Physical Sciences (MOE), State Key Laboratory of Surface Physics, and Department of Physics, Fudan University, Shanghai 200433, China*

<sup>†</sup> *Collaborative Innovation Center of Advanced Microstructures, Nanjing 210093, China*

<sup>‡</sup> *Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Zum Gro ß en Windkanal 6, D-12489 Berlin, Germany*

<sup>4</sup> *Department of Physics, and International Center of Quantum and Molecular Structures, Shanghai University, Shanghai 200444, China*

<sup>5</sup> *CNR-SPIN, Via Vetoio, L' Aquila 67100, Italy*

Hybrid organic-inorganic compounds attract a lot of interest for their flexible structures and multi-functional properties. For example, they can have coexisting magnetism and ferroelectricity whose possible coupling gives rise to magnetoelectricity. Here using first-principles computations, we show that, in a perovskite metal-organic framework (MOF), the magnetic and electric orders are further coupled to optical excitations, leading to an Electric tuning of the Magneto-Optical Kerr effect (EMOKE). Moreover, the Kerr angle can be switched by reversal of both ferroelectric and magnetic polarization only. The interplay between the Kerr angle and the organic-inorganic components of MOFs offers surprising unprecedented tools for engineering MOKE in complex compounds. Note that this work may be relevant to acentric magnetic systems in general, e.g., multiferroics.

[1] *J. Am. Chem. Soc.* 2017, 139, 37, 12883-12886

---

## Electronic structure of perfect and imperfect cubic carbides

P16

Mehdi Nourazar\* and Pavel Korzhavy<sup>†</sup>

\* *Department of Material Science and Engineering, KTH-Royal Institute of Technology, SE-100 44 Stockholm, Sweden*

<sup>†</sup> *Department of Material Science and Engineering, KTH-Royal Institute of Technology, SE-100 44 Stockholm, Sweden*

We employ first-principles to study the electronic and atomic structure of various defects, defect interactions, and defect arrangements in the main phases of transition metal carbides.

These studies are to provide data on the atomic-level structures and mechanisms that are important for understanding and controlling the thermodynamic, mechanical, and kinetic properties. We adopt an integrated computational modeling approach, based on quantum mechanics and statistical physics. Starting from electronic and atomic levels and passing the data to semi-discrete and continuum methods that operate at longer length and time scales. Within this approach, our group has developed efficient theoretical tools for describing the thermodynamic and kinetic properties of materials at elevated temperatures.

These methods enable computer-aided optimization of the compositions and the heat treatment regimes of new grades of steel, superalloys, and refractory ceramics, with the goal to adapt these materials to novel applications in which an unusual combination of properties may be required.

- [1] Ehteshami, H., Ruban, A. V., Korzhavyi, P. A. (n.d.). Role of defects in Ti(O,C). Retrieved from <http://urn.kb.se/resolve?urn=urn:nbn:se:kth:diva-223666>
- [2] Structure and energy of point defects in TiC: An ab initio study W Sun, H Ehteshami, PA Korzhavyi - Physical Review B, 2015

---

## Energetics and structure of Langmuir monolayers of palmitic acid: a DFT study

P17

Óscar Toledano Sanz\* and Óscar Gálvez González\*

\* *Departamento de Física Interdisciplinar, Fac. de Ciencias, Universidad Nacional de Educación a Distancia (UNED), Madrid, Spain*

Langmuir monolayers are monomolecular wide films composed of amphiphilic molecules with a bi-dimensional structure typically formed at the air-water interface. They have been studied for many years because these monolayers have important applications in many research fields [1]. Their phases diagram present several condensed phases whose atomic structure is not yet completely known. We present a novel density functional study on palmitic acid dimers and monolayers. Our results reveal that dihydrogen bond interactions established among alkyl chains play a leading role in the final structure, regarding both dimers and for the arrangement of molecules in the monolayer. In addition, our calculations show that tilted phases at approx. 30° can be formed without significant loss of structure stability, a result that is in agreement with the experimental findings [2]. Different structures for the high pressure phases, S and CS, are proposed here for the first time, being in good agreement with the diffraction data available. Furthermore, linear compressibility values also in accordance with previous experimental studies [3] are presented for several structures.

- [1] F. Schreiber, Progress in Surface Science, 2000, 65, 151 – 256.
- [2] V. M. Kaganer, H. Möhwald, P. Dutta, Reviews of Modern Physics, 1999, 71, 779-819.
- [3] C. Fradin, J. Daillant, A. Braslav, D. Luzet, M. Alba and M. Goldman, The European Physical Journal B, 1998, 1, 57-69.

---

## Scattering of Hydrogen Atoms at $\alpha$ -Al<sub>2</sub>O<sub>3</sub> Surfaces

P18

Martin Liebetrau\* and Jörg Behler\*

\* *Theoretische Chemie, Universität Göttingen, Tammannstr. 6, 37077 Göttingen, Germany*

The adsorption of atomic hydrogen is important in many fields, from heterogeneous catalysis to interstellar hydrogen on dust grains and nuclear fusion. Recently, an experimental work investigated high-energy hydrogen atom scattering at  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>. [1] Here, we report molecular dynamics simulations of this system investigating a signal loss in the experiment at higher kinetic energies. Employing a high-dimensional neural network potential, [2] which allows us to include the full-dimensional thermal motion of the surface atoms, we are able to calculate a large number of trajectories with the accuracy of density-functional theory. Probing different kinetic energies and incident angles, we are able to characterize the interaction with the surface in detail.

[1] Dorenkamp, Y., C. Volkmann, V. Roddatis, S. Schneider, A.M. Wodtke, O. Buenermann, *J. Phys. Chem. C* **122** (2018) 10096-10102.

[2] J. Behler, *Angew. Chem. Int. Ed.* **56** (2017) 12828-12840.

---

## Morphological Changes in Nafion under Confinement and Protonation State/pH Variation

P19

Soumyadipta Sengupta\*,† and Alexey Lyulin\*,‡

\* *TU Eindhoven*† *NWO*‡ *CCER*

Nafion is a commonly used polyelectrolyte membrane in fuel cells and flow batteries. Nanocomposites of Nafion are used to enhance properties like electrolyte selectivity, temperature resistance and conductivity. Nafion nanocomposites have been modelled using a Nafion film confined between two potential walls representing variable wettability and have been simulated using classical atomistic molecular dynamics (MD) [1]. The average water cluster sizes in the Nafion films decreased with increasing wall wettability and also with decreasing film thickness at any fixed wall wettability. This qualitatively matched with experimental Nafion- modified GO nanocomposite water phase morphology changes and Nafion film SAXS results. Previous experiments [2] have shown that Nafion protonation states vary significantly with hydration levels. The different protonation states of Nafion has been simulated using classical MD. The water domains sizes decreased with increasing deprotonation/solution pH while the average water cluster sizes increased at the same time for any fixed protonation state. This meant that the water clusters were becoming narrower and longer with increasing solution pH. This matched very well with shape changes of in situ platinum nanoparticles deposited inside hydrated Nafion with pH variation [3].

[1] Sengupta et al., *J.Phys.Chem.B*, May 2018, pg 6107-6119

[2] Spry et al., *J.Phys.Chem.B*, July 2009, pg 10210-10221

[3] Ingle et al., *Langmuir*, Feb 2014, pg 1871 – 1879

---

## Stability and Electronic Properties of the Palladium Dichalcogenides as Nanomaterials

P20

Roman Kempt\*, Agnieszka Kuc\* and Thomas Heine\*,†

\* *Helmholtz-Zentrum Dresden-Rossendorf, Germany*† *TU Dresden, Germany*

The palladium dichalcogenides PdX<sub>2</sub> have attracted a lot of recent attention due to their unique structural features, superior gas-sensing properties and excellent carrier mobilities, as well as possible Type-II Dirac fermions. We present a detailed computational investigation of their stability and electronic properties as bulk and nanomaterials. There, we focus on the PdS<sub>2</sub>-type polymorph with pentagonal Cairo-type lattice, the pyrite-type structure and the CdI<sub>2</sub>-type structure, and how these might be transformed into one another. Furthermore, we investigate their ternary mixtures to tune stabilities and properties. We show that it requires a hybrid approach to account for local and non-local exchange and correlation effects in these systems to properly model their structures and stabilities.

- [1] F. Grønbold, E. Røst, *Acta Crystallogr.* 1957, 10, 32.
- [2] A. D. Oyedele et al., *J. Am. Chem. Soc.* 2017, 139, 14090.
- [3] Chow, W. L. et al., *Adv. Mater.* 2017, 29, 1602969.
- [4] Fucong Fei et al., *Phys. Rev. B* 96, 041201(R).

---

## Analysis of peptide-chains and transport properties of polar amino-acids chains of different size.

P21

Tommaso Civitarese\*

\* *Tommaso Civitarese, S.B.A.I. department, Sapienza University of Rome.*† *Aldo Eugenio Rossini, S.B.A.I. department, Sapienza University of Rome.*‡ *Giuseppe Zollo, S.B.A.I. department, Sapienza University of Rome.*

The importance of identifying the sequence and the 3-D structure of proteins is crucial to understanding their function and behavior within living organisms; for instance, mis-folding of proteins is believed to be related to neurodegenerative diseases such as Parkinson's and Alzheimer. Current methods require long sequencing times that represent a serious bottleneck for the needs of the rising importance of proteomics. Then fast and efficient techniques (especially for large protein chains) are required and solid-state nanopores and nanogaps are emerging as promising tools for single molecule analysis [1,2,3]. In this framework, a new sequencer consisting of arrays of nano-gaps between graphene nano-ribbons is proposed[4]: the atomistic resolution provided by the measuring of the transverse current permits, in principle, to recognize the specific peptide bond which is located between the two leads. A DFT-based ab initio study, in conjunction with the Non Equilibrium Green Function (NEGF) method[5,6] and the Landauer-Büttiker approach[7] has evidenced clear peptide bond fingerprints made of two, well defined current peaks of the order of magnitude

of  $nA$  in the case of glycine poly-peptides translocating across the gap[4]. Besides depending on the graphene nano-ribbon chirality[8], the tunneling current signals should also be closely related to the amino-acids size and polar state. Then we have analyzed the transmission properties of various graphene nano-gaps and we have studied asparagine (Asn) and threonine (Thr) poly-peptides to explore the effects of polar side chains of different size on the transverse current calculation.

- [1] G. Goyal, Y. B. Lee, A. Darvish, C. W. Ahn and M. J. Kim, *Nanotechnology*, 2016.
- [2] F. Traversi, C. Raillon, S. Benameur, K. Liu, S. Khlybov, M. Tosun, D. Krasnozhan, A. Kis and A. Radenovic, *Nat. Nanotechnol.*, 2013.
- [3] J. Prasongkit, G. T. Feliciano, A. R. Rocha, Y. He, T. Osotchan, R. Ahuja and R. H. Scheicher, *Sci. Rep.*, 2015.
- [4] Rossini, Aldo Eugenio, et al. "Peptide bond detection via graphene nanogaps: a proof of principle study." *Nanoscale* 10.13, 2018.
- [5] J. Soler, E. Artacho, J. Gale, A. García, J. Junquera, P. Ordejón and D. Sánchez-Portal, *J. Phys.: Condens. Matter*, 2002.
- [6] K. Stokbro, J. Taylor, M. Brandbyge and P. Ordejón, *Ann. N. Y. Acad. Sci.*, 2003.
- [7] Landauer, R., *IBM Journal of Research and Development*, 1957.
- [8] Li, Zuanyi, et al *Physical review letters*, 2008.

---

## Understanding Alloys and Metal Sulfides as Electrocatalysts for Nitrate Reduction

P22

Samuel Young\*, Jin-Xun Liu\*, Zixuan Wang\*, Danielle Richards\*, Nirala Singh\* and  
Bryan Goldsmith\*  
\* *University of Michigan*

Nitrate ( $\text{NO}_3^-$ ) is one of the most prevalent water pollutants [1]. Elevated  $\text{NO}_3^-$  levels lead to eutrophic "dead zones", and to methemoglobinemia and various cancers via human consumption [2]. Current remediation technologies (e.g., filtration and biological consumption) produce secondary waste streams (e.g., concentrated nitrate or bacteria) requiring further treatment [3,4]. An alternative is the electrocatalytic nitrate reduction reaction ( $\text{NO}_3\text{RR}$ ), which produces no waste stream, could run on renewable electricity, and could treat waste too toxic for bacteria. We propose a computational study to better understand how the  $\text{NO}_3\text{RR}$  reduces  $\text{NO}_3^-$  to desirable products ( $\text{N}_2$  and  $\text{NH}_3$ ) on platinum group metal (PGM) alloy and rhodium sulfide ( $\text{Rh}_x\text{S}_y$ ) catalysts. Many PGM alloys have  $\text{NO}_3\text{RR}$  activities and selectivities superior to their pure-metal counterparts, but reasons for this are poorly understood. We also consider  $\text{Rh}_x\text{S}_y$  catalysts, which have not yet been explored for the  $\text{NO}_3\text{RR}$ , but demonstrate poison resistance to the halide ions present in many waste streams [5].

Our work will use density functional theory (DFT), microkinetic modelling, and active machine learning (AML) to search the PGM alloy and  $\text{Rh}_x\text{S}_y$  materials space for active and selective  $\text{NO}_3\text{RR}$  catalysts. We first use DFT modeling to study  $\text{NO}_3^-$  binding energy trends, adsorbate scaling relationships, and Brønsted-Evans-Polanyi relationships. We then apply microkinetic modelling to predict catalyst selectivity towards desired products and an AML framework to build an ensemble of surrogate models for catalyst performance. Our AML framework will use uncertainty sampling with both exploration and exploitation to search among many thousands of possible catalysts for the most promising materials. Such studies would be infeasible using DFT modeling only.

Ultimately, our work will help engender rational design of selective and active NO<sub>3</sub>RR catalysts and enable more robust denitrification. Additionally, the further development of an AML catalyst discovery framework will enable more rapid and effective design of many environmentally important catalysts, and yield insight into previously unstudied reaction mechanisms.

- [1] Burow, K. R. et al. *Environ. Sci. Technol.* **2010**, *44* (13), 4988–4997.
- [2] Gruber, N et al. *Nature* **2008**, *451* (7176), 293–296.
- [3] Duca, M. et al. *Energy Environ. Sci.* **2012**, *5* (12), 9726–9742.
- [4] Song, H. et al. *J. Desalination* **2012**, *296*, 53–60.
- [5] Ziegelbauer, J. M. et al. *Electrochimica Acta* **2007**, *52* (21), 6282–6294.

## Benchmarking $G_0W_0$ calculations for open-shell molecules

P23

Masoud Mansouri<sup>\*,†</sup>, Peter Koval<sup>\*,‡</sup> and Daniel Sánchez-Portal<sup>\*,†</sup>

<sup>\*</sup> *Donostia International Physics Center (DIPC), Lardizabal 4, San Sebastián, Spain*

<sup>†</sup> *Centro de Física de Materiales, Centro Mixto CSIC-UPV/EHU, Lardizabal 5, San Sebastián, Spain*

<sup>‡</sup> *Simune Atomistics S.L., Av. de Tolosa 76, San Sebastián, Spain*

Hedin’s  $GW$  approximation ( $GWA$ ) has gained popularity in the material science community because of its high quality and relatively low computational cost. A prerequisite to describe magnetic materials is the capability to describe systems containing unpaired electrons.

In this study, we benchmark the ionization potential (IP) calculated by unrestricted  $G_0W_0$  on top of different starting points for 42 small molecules belonging to the G2/97 test set using Dunning’s correlation-consistent basis sets expanded in terms of Gaussian functions. In order to examine the validity of the implemented approach, calculated IPs are compared with a variety of correlated methods in the  $\Delta$ SCF framework including the gold standard in quantum chemistry, namely CCSD(T). The results revealed that  $G_0W_0$  provides a systematic and accurate method to compute the quasi-particle energy levels of open-shell molecules with convincing evidence of reliability similar to the case of closed-shell molecules[1-3].  $GWA$  provides the correct ordering of the molecular orbitals, in particular, for all the studied molecules we obtained the HOMO level with the right character. The present implementation of  $GWA$  is based on the use of basis sets of atomic orbitals and provides a good compromise between accuracy and computational expense, suitable to be applied to study magnetic materials.

Keywords:  $G_0W_0$  Approximation, Numerical Atomic Orbital, Ionization Potential.

Authors acknowledge support from Spanish MINECO Grants MAT2016-78293-C6-4-R and RTC-2016-5681-7 (SIESTA-PRO).

- [1] Fabien Bruneval and et al. "Benchmarking the starting points of the GW approximation for molecules"; *Journal of chemical theory and computation*, 9(1):324 – 329, 2012.
- [2] Joseph W Knight, and et al. "Accurate ionization potentials and electron affinities of acceptor molecules III: a benchmark of GW methods"; *Journal of chemical theory and computation*, 12(2):615 – 626, 2016.
- [3] Michiel J van Setten, and et al. "GW 100: Benchmarking GW for molecular systems"; *Journal of chemical theory and computation*, 11(12):5665 – 5687, 2015.



---

## Investigation of the Elastic Properties of Binary Alloys through a mixed modelling-experimental approach

P24

Paul Stavroulakis\*, Dr. Colin Freeman\* and Dr. Russell Goodall\*

\* *The University of Sheffield*

First-principles calculations are widely used to study materials with the aim to gain a better understanding of complex behaviours and in the case of metallurgy, to allow for better alloy design. The current objective of this work is the study of binary alloying systems from both a modelling and experimental perspective with a view to future application to high entropy alloys (HEAs) [1, 2]. The simulations, using Density Functional Theory (DFT) with CASTEP [3], explore the crystallographic characteristics and subsequently the elasticity constants for Cu-Ni and Ti-Nb systems. In parallel, the results of the simulations are experimentally evaluated with samples cast using Vacuum Arc Melting (VAM). The chemical composition of the samples is verified through X-Ray Fluorescence (XRF). The crystal structure and lattice parameters of the as-cast alloys is determined through X-Ray Diffraction (XRD) analysis. Lastly, the elastic constants are measured through nanoindentation, while the microstructural characteristics and the homogeneous distribution of alloying elements is evaluated using Optical Microscopy (OM), Scanning Electron Microscopy (SEM) and Energy-dispersive X-Ray Spectroscopy (EDS) analysis. The results to date and the perspectives for future developments will be discussed within this presentation.

- [1] S. Huang et. al., Elasticity of high-entropy alloys from ab initio theory. *J. Mat. R.*, 33 (19), 2018, pg. 2938-2953.
- [2] E. J. Pickering, N. G. Jones, High-entropy alloys: a critical assessment of their founding principles and future prospects. *Int. Mat. Rev.*, 61 (3), 2016, pg. 183-202.
- [3] S. J. Clark et. al., First principles methods using CASTEP. *Zeitschrift für Kristallographie*, 220, 2005, pg. 567-570.

---

## Electronic Structure and Lithium Storage Mechanism of Niobium Oxide-based Crystallographic Shear Phases from First Principles

P25

Can P. Koçer\* and Andrew J. Morris†

\* *Theory of Condensed Matter Group, Cavendish Laboratory, University of Cambridge*

† *School of Metallurgy and Materials, University of Birmingham*

Crystallographic shear phases of niobium oxide have shown unprecedented high-rate performance as high-voltage anodes for lithium ion batteries [1]. The electronic structure, lithium insertion mechanism, and lithium dynamics of these compounds remain relatively unexplored, due to their novelty and complexity. I will present recent first-principles studies on the electronic structure and lithium insertion mechanism of crystallographic shear phases in the Wadsley-Roth family. Our work has explored interesting electron localisation-delocalisation transitions on *n*-type doping in the

niobium suboxides [2], and provides a unified mechanistic picture for the structural changes during lithium insertion in the entire family of crystallographic shear phases [3]. I will discuss challenges associated with modelling these materials, and will point out future directions for experimental and first-principles studies.

- [1] K. J. Griffith et al., *Nature* 559, 556-563 (2018)
- [2] C. P. Koçer et al., *Phys. Rev. B*, 99, 075151 (2019)
- [3] C. P. Koçer et al. (in preparation)

## MRChem for crystalline systems

P26

Magnar Bjørgve<sup>\*,†</sup>, Stig Rune Jensen<sup>\*,†</sup> and Luca Frediani<sup>\*,†</sup>

<sup>\*</sup> *UiT The Arctic University of Norway*

<sup>†</sup> *Hylleraas Centre for Quantum Molecular Sciences*

MRChem is a numerical real-space code for molecular electronic structure calculations within the self-consistent field (SCF) approximation of quantum chemistry, capable of performing Hartree-Fock and Density Functional Theory calculations. Contrary to most mainstream programs, it uses a multiwavelets (MWs) as a basis, due to their mathematical properties, such as error control and reduced scaling. The code has recently been applied to two large and precise benchmark studies on electronic energies[1] and magnetizabilities and shielding constants[2].

We are currently expanding the code to solve the Kohn-Sham equations for crystalline systems. We give an overview of this work including examples of total energies compared with other solid state codes, and how MWs can be used to systematically increase the accuracy of the result with respect to the basis set.

- [1] S. R. Jensen, S. Saha, J. A. Flores-Livas, W. Huhn, V. Blum, S. Goedecker, and L. Frediani, *J Phys Chem Lett* 8, 1449-1457 (2017).
- [2] S. R. Jensen, T. Fla, D. Jonsson, R. S. Monstad, K. Ruud, and L. Frediani, *Phys Chem Chem Phys* 18, 21145-21161 (2016).

## Time-resolved transport in quantum optoelectronic nanodevices

P27

Katawoura Beltako<sup>\*,†</sup>, Nicolas. Cavassilas<sup>\*</sup>, Fabian Pauly<sup>†</sup> and Fabienne Michelini<sup>\*</sup>

<sup>\*</sup> *Aix-Marseille University, CNRS, IM2NP, UMR 7334, 13288 Marseille, France*

<sup>†</sup> *Okinawa Institute of Science and Technology Graduate University, Onna-son, Okinawa 904-0395, Japan*

Recent advances in excitation frequencies beyond gigahertz offer the ability to probe the fast internal response of a quantum system. Time dependence in nanoelectronics constitutes a major challenge for the next advances in device modeling and simulations. Oscillating gate voltages, time-dependent

bias but also applied illumination pulses all are examples of key issues in quantum transport simulations, which require novel approaches as well as efficient numerical methods. In this context we proposed a suitable technique and efficient algorithms to the simulation of time-dependent transport in nano-systems interacting with light radiation [1],[2], relying on state of the art quantum statistical methodologies. The method uses the formalism of non-equilibrium Green's functions, and the developed algorithms have enabled us to investigate dynamical carrier transfer processes in molecular nanojunctions. The study elucidated intra-molecular tunneling oscillations, excitons induced molecular orbitals reorganization and inspired experimental proposals for the measurement of internal quantum characteristics of these molecular junctions such as intra-molecular couplings. Even though more accurate simulations should account for the full electronic structure calculation from advanced ab initio methods, the technique gives an insight into the relevance of transient dynamics in the understanding of time-resolved optoelectronic nanodevice operations. The work provides us with a valuable tool for ultrafast quantum transport simulation.

[1] Selzer, Y.; Peskin, U. *J. Phys. Chem. C* 2013, 117, 22369 – 22376

[2] Gaury, B.; Weston, Waintal and co-workers, *X. Physics Reports* 2014, 534, 1 – 37

## Theoretical Design of Two-Dimensional Magnetoelectric materials

P28

Shuai Dong\*

\* *School of Physics, Southeast University*

Achieving magnetoelectric two-dimensional (2D) materials should enable numerous functionalities in nanoscale devices. Until now, however, predicted 2D magnetoelectric materials are very few and with coexisting yet only loosely coupled (type-I) ferroelectricity and magnetism [1]. Based on physical analysis and by using density functional theory calculations, a type-II multiferroic MXene Hf<sub>2</sub>VC<sub>2</sub>F<sub>2</sub> monolayer is predicted. For multiferroic MXene Hf<sub>2</sub>VC<sub>2</sub>F<sub>2</sub> monolayer, its ferroelectricity originates directly from its magnetism [2]. The noncollinear 120° Y-type spin order generates a polarization perpendicular to the spin helical plane. Remarkably, the multiferroic transition is estimated to occur above room temperature. Our investigation should open the door to a new branch of 2D materials in the pursuit of intrinsically strong magnetoelectricity.

[1] Y.H. Zhao, L.F. Lin, Q.H. Zhou, Y.H. Li, S.J. Yuan, Q. Chen, S. Dong, J.L. Wang, *Nano Letters* 18, 2943 (2018).

[2] J.-J. Zhang, L.F. Lin, Y. Zhang, M.H. Wu, B. Yakobson, S. Dong, *J. Am. Chem. Soc.* 140, 9768 (2018).

## Transport through nanostructures within the GW scheme

P29

León-Alexander Martín<sup>\*,†</sup> and Fabian Pauly<sup>\*,†</sup>

\* *University of Konstanz*

† *Okinawa Institute of Science and Technology*

Starting from calculations for the electronic structure with density-functional theory (DFT), a non-equilibrium Green's functions (NEGF) approach can be used to calculate the electronic transport through atomic and molecular contacts without system-dependent parameters [1]. However, since electronic quasiparticle energies computed with DFT are not very accurate, transport calculations typically differ from experiments [2]. Accuracies can be improved by determining the electronic structure with the GW method [2], which is based on many-body perturbation theory (MBPT) and the Hedin's equations [3] and has been shown to be successful in describing the electronic structure of various systems ranging from molecules to wires, two-dimensional sheets and bulk solids. First attempts indeed demonstrated that transport through single-molecule contacts is better described with the GW scheme compared to those based on DFT [4,5]. However, due to its high computational cost this procedure has not yet become the state of the standard in the field of molecular electronics. Here we show new studies of GW-based transport through molecular junctions, which are based on recent developments of the GW implementation in TURBOMOLE [6].

- [1] J. C. Cuevas et al., *Nanotechnology* 14, R29 (2003)
- [2] M. Thoss, F. Evers, *J. Chem. Phys.* 148, 030901 (2018)
- [3] L. Hedin, *Phys. Rev.* 139, A796 (1965)
- [4] M. Strange et al., *Phys. Rev. B* 83, 115108 (2011)
- [5] T. Rangel et. al., *Phys. Rev. B* 84, 045426 (2011)
- [6] F. Kaplan et al., *J. Chem. Theory Comput.* 12, 2528 (2015)

---

## Ab-initio quantum transport through atomic and molecular junctions

P30

Yuta Ito\*, Werner M. Schosser\*,<sup>†</sup> and Fabian Pauly\*,<sup>†</sup>

\* *Okinawa Institute of Science and Technology Graduate University, Okinawa 9040412, Japan*

<sup>†</sup> *University of Konstanz, Konstanz 78464, Germany*

A frequently used procedure to study phase-coherent transport through atomic and molecular junctions is the combination of density functional theory (DFT) with the nonequilibrium Green's function (NEGF) technique [1,2]. To complete this procedure, it is necessary to construct surface Green's functions from bulk parameters to describe the electrodes. Such bulk parameters can be extracted from large clusters or through calculations with periodic boundary conditions. In this work we explore the differences in charge transport between our previous cluster-based approach [2] and newly available functionalities for periodic systems in the quantum chemistry package TURBOMOLE [3].

- [1] M. Brandbyge, J.-L. Mozos, P. Ordejón, J. Taylor, K. Stokbro, *Phys. Rev. B* 65, 165401 (2002)
- [2] F. Pauly, J. K. Viljas, U. Huniar, M. Häfner, S. Wohlthat, M. Bürkle, J. C. Cuevas, G. Schön, *New J. Phys.* 10, 125019 (2008)
- [3] R. Łazarski, A. M. Burow, L. Grajciar, M. Sierka, *J. Comput. Chem.* 37, 2518 (2016)

---

## A transferable machine-learning model for full-electron charge densities

P31

Andrea Grisafi\*, Alberto Fabrizio<sup>†,‡</sup>, Benjamin Meyer<sup>†,‡</sup>, David Wilkins\*,  
Clemence Corminboeuf<sup>†,‡</sup> and Michele Ceriotti<sup>\*,‡</sup>

\* *Laboratory of Computational Science and Modeling, IMX, EPFL, Lausanne*

† *Laboratory for Computational Molecular Design, ISIC, EPFL, Lausanne*

‡ *National Centre for Computational Design and Discovery of Novel Materials*

We propose an effective and transferable learning model for the ground-state electron density of a system. Using the nuclear coordinates as the sole input, this framework can in principle be used on arbitrarily complex systems, where no prior knowledge is assumed about the underlying molecular geometry [1]. The model reaches a similar accuracy as that obtained by Brockherde *et al.* [2], but is substantially more transferable thanks to the combination of an atom-centered basis set to represent the electron density and the possibility of predicting the local density components in a symmetry-adapted fashion [3]. A major consequence is that accurate linear-scaling extrapolations of the electron density can be obtained for systems much larger than those used to train the model. Improving on the method introduced in Ref.[1], we show how using a resolution of the identity basis set [4] makes it possible to predict the full-electron charge density of molecular systems across a large spectrum of chemical diversity.

[1] Grisafi et al., ACS Central Science, **5**, 57 (2019)

[2] Brockherde et al., Nature Communications, **8**, 872 (2017)

[3] Grisafi et al., Physical Review Letters, **120**, 036002 (2018)

[4] C. Hättig, Physical Chemistry Chemical Physics, **7**, 59 (2005)

---

## Predicting molecular conformers using Machine Learning

P32

Carlos Manuel de Armas Morejon<sup>\*,†</sup>, Phd. Joaquim Jornet Somosa<sup>‡</sup>, Phd. Ask Hjort Larsen\*,  
Prof. Dr. Sc. Luis A. Montero-Cabrera<sup>†</sup> and Prof. Dr. Angel Rubio<sup>\*,‡</sup>

\* *UPV/EHU University of the Basque Country, Spain*

† *UH University of Havana, Cuba*

‡ *Max Planck Institute, Hamburg, Germany*

One of the most attractive fields of science today are machine learning (ML) algorithms.[1], [2] They are being applied to almost every branch of knowledge, and chemistry is not an exception. In this work, we propose a method to find stable molecular geometries. Accurate geometry optimization requires the use of computationally expensive *ab initio* or DFT methods, and a good initial geometry is essential. We propose a ML approach to find conformations by predicting the local arrangement of each atom belonging to the molecule using a database of optimized small molecules. We train the algorithm by dividing each molecule in the database[3] into minimal "building blocks" using an electro-topological[4] fingerprint as descriptor. For a given connectivity matrix we can then predict molecular conformers. Results promise fast and accurately predictions of molecular geometries and conformations from their formulas as structural graphs.

- [1] Butler et al., Nature, 2018, 559, 547.
- [2] Chmiela et al., Science Advances 2017, 3, 5.
- [3] Ramakrishnan et al., The Journal of Chemical Physics 2015, 143, 084111.
- [4] H. Hall et al., J. Chem. Inf. Comput. Sci., 1995, 35 (6), pp 1039 – 1045

---

## Frustrated Structure Instability and Magnetism of superconducting KCr3As3

P33

Guangzong Xing<sup>\*,†</sup>, David J. Singh<sup>†</sup> and Fabian Pauly<sup>\*</sup>

<sup>\*</sup> *Okinawa Institute of Science and Technology Graduate University*

<sup>†</sup> *Department of Physics and Astronomy, University of Missouri, Columbia*

We find a lattice instability in the superconductor KCr3As3 [1 – 3] using first-principles calculations based on density functional theory (DFT), corresponding to a distortion of the Cr metallic wires in the crystal structure. The energy gain from the distortion is 0.15 eV per formula unit, which is a very sizable energy that is well outside of the range expected for DFT errors and is also much larger than the magnetic energies for the ideal structure. Phonon calculations with the finite difference supercell method [4] shows that modes at the  $\Gamma$  point are unstable. However, these unstable modes do not exist in the distorted structure, indicating that our reported distorted structure is dynamically stable. This distortion couples strongly to both the electronic and magnetic properties, in particular by making the electronic structure nearly one-dimensional, and by shifting the compound away from magnetism. We discuss the implications of this results in the context of the possibly unconventional superconductivity of this phase.

- [1] Q.-G. Mu et al. Phys. Rev. B 96, 140504 (2017).
- [2] J.-K. Bao et al. Phys. Rev. B 91, 180404 (2015).
- [3] C. Cao et al. Phys. Rev. B 92, 235107 (2015).
- [4] A. Togo and I. Tanaka, Scr. Mater. 108, 1 (2015).

---

## One Million Crystal Structures: One Million Disappearing Polymorphs Waiting to Happen?

P34

Asbjoern M. Burow<sup>\*</sup>, Jacco van de Streek<sup>\*</sup> and Marcus A. Neumann<sup>\*</sup>

<sup>\*</sup> *Avant-garde Materials Simulation Deutschland GmbH, Alte Strasse 2, D-79249 Merzhausen*

On rare occasions, a crystal structure that has been prepared for years is unexpectedly "superseded" by a thermodynamically more stable polymorph, rendering the initial crystal structure almost impossible to obtain – a so-called "disappearing polymorph" [1].

On a case-by-case basis, the probability of a kinetically hindered but thermodynamically stable polymorph having been missed in an experimental polymorph screen can be assessed by a computational crystal structure prediction (CSP) study: the calculations do not suffer from kinetics

and will in principle enumerate all possible crystal structures for a given compound; comparison against the experimental structures identifies any missed polymorphs. In a recent paper, two of us presented the results of 41 such computational CSP studies to draw up statistics regarding the number of hidden disappearing polymorphs [2]. The main finding of the paper was that between 15 and 45 % of all experimental crystal structures are in fact thermodynamically unstable. The large spread of this estimate was due to the computational error in the calculation of the relative free energies. Even though the computational error is estimated to be as small as 0.5 kcal/mol, about half the size of the gold standard referred to as "chemical accuracy", the experimental energy differences between polymorphs are also around the 0.5 kcal/mol mark, and to reduce the large spread in our estimate an even more accurate energy model was needed.

The shortcomings of our old energy model – neglect of temperature, relatively poor accuracy of the exchange part of the functional used in the DFT calculations, and the assumption that Van der Waals interactions are pairwise additive – are well documented, and in this contribution we will present the results of an energy model in which these shortcomings have been addressed [3]. With the availability of more accurate relative lattice energies, we are able to narrow down our estimate of how many of the one million experimental crystal structures represent a thermodynamically unstable polymorph at ambient conditions.

- [1] D.-K. Bučar, R. W. Lancaster, and J. Bernstein (2015), *Angew. Chem., Int. Ed.* **54**, 6972-6993.
- [2] M. A. Neumann and J. van de Streek (2018), *Faraday Discuss.* **211**, 441-458.
- [3] J. Hoja, Hsin-Yu Ko, M. A. Neumann, R. Car, R. A. DiStasio Jr., and A. Tkatchenko (2019), *Sci. Adv.* **5**, eaau3338.

---

## Modelling lithium intercalated graphite on the basis of semi-empirical electronic structure simulations with machine learning elements

P35

Simon Anniés\*, Chiara Panosetti\*, Christoph Scheurer\* and Karsten Reuter\*  
\* *TU Munich*

Lithium ion batteries have been a central part of consumer electronics for multiple decades. More recently, they have also become one of the fundamental components on which the quickly arising technological fields of sustainable electric transportation and renewable energy sustenance are based. However, many core principles and mechanisms are not yet understood to a sufficient extent to fully realize the potential of the incorporated materials.

The vast majority of lithium ion batteries make use of graphite anodes [1], the functionality of which is governed by the process of *intercalation* – the embedding and ordering of (lithium-) ions in the two-dimensional spaces between the graphene sheets. This important process – it yields the upper bound to a battery’s charging speed and plays a decisive role for its longevity – is characterized by multiple phase-transitions, ordered and disordered domains, as well as non-equilibrium phenomena, and therefore quite complex.

In this work, we provide a simulation-framework for the purpose of better understanding lithium intercalated graphite and its behaviour during use in a battery. In order to address the large scale

of systems and long time frames needed to investigate said effects, we combine the highly efficient, but semi-empirical Density Functional Tight Binding (DFTB [2]) approach with the machine learning based Gaussian Process Regression (GPR [3]). Using the resulting parametrization, we are able to reproduce experimental reference structures at a level of accuracy which is in no way inferior to much more costly *ab initio* methods. Reassured by this success, we finally present structural properties and diffusion barriers for a wide variety of possible system states and discuss the trends discovered therein.

- [1] N. Nitta, F. Wu, J. T. Lee, and G. Yushin, "Li-ion battery materials: present and future", *Materials today*, vol. 18, no. 5, pp. 252-264, 2015
- [2] M. Elstner, D. Porezag, G. Jungnickel, J. Elsner, M. Haugk, T. Frauenheim, S. Suhai, and G. Seifert, "Self-consistent-charge density-functional tight-binding method for simulations of complex materials properties", *Phys. Rev. B*, vol. 58, pp. 7260-7268, 1998
- [3] A. Engelmann, "The generation of pairwise interatomic potentials from arbitrary structures - a machine learning approach with application in dftb", Master's thesis, Technical University Munich, 2018

---

## Computational Investigations of Ultrasmall Titanium Dioxide Nanoparticles

P36

John Lasseter<sup>\*,†</sup>, David Geohegan<sup>\*</sup>, Mina Yoon<sup>\*</sup> and Erik Inclan<sup>\*</sup>

<sup>\*</sup> *Center for Nanophase Materials Science, Oak Ridge National Lab*

<sup>†</sup> *College of Basic and Applied Sciences, Middle Tennessee State University*

Using a pulsed-laser deposition technique, ultrasmall, nanometer-scale TiO<sub>2</sub> structures have been synthesized in the lab. They are interesting for potential applications but need theoretical understanding of their basic structural and electronic properties. We investigated clusters, (TiO<sub>2</sub>)<sub>n</sub>, consisting of n=1-50 TiO<sub>2</sub> units. Using the structures that were generated using a global structure search algorithm, we performed structure optimization employing first-principle quantum mechanical calculations as implemented in the VASP (Vienna Ab initio Simulation Program) software package. We then further analyze for their structures, structural stabilities, and electronic properties. Our results show the expected convergence to bulk material characteristics as the cluster size increases. The nanoclusters trended toward compact, low surface area structures that share characteristics of the bulk, namely the formation octahedral microstructures as the nanoclusters increased in size. Our study helps in better identifying and characterizing experimentally observed structures.

- [1]



---

## Multiscale Modeling of Interface Effects on the Redox Chemistry of Ceria Nanoparticles

P37

Byung-Hyun Kim<sup>\*,†</sup>, Matthew J. Wolf<sup>†,‡</sup>, Jolla Kullgren<sup>†</sup>, Kersti Hermansson<sup>†</sup> and Peter Broqvist<sup>†</sup>

<sup>\*</sup> Platform Technology Laboratory, Korea Institute of Energy Research

<sup>†</sup> Department of Chemistry – Ångström Laboratory, Uppsala University

<sup>‡</sup> Department of Physics, University of Bath

Synthesized ceria samples often appear in the form of agglomerates of nanoparticles (NPs) [1,2]. Only a small fraction of the numerous published studies in recent years have carefully examined. To the best of our knowledge, detailed theoretical investigations at the atomic scale of ceria NP interfaces and their redox activity are lacking in the scientific literature. In the present study, the interface stability and its effects on redox properties in agglomerated ceria nanoparticles have been investigated using a sequential multiscale simulation approach linking three levels of theory along the multiscale ladder, Hubbard augmented DFT [3-6], self-consistent-charge density functional tight binding [7-9] and a DFT-parameterized reactive force-field [10, 11]. We will present the stable ceria interface structures found and their effects on the oxygen vacancy formation energy, which we will use as a key descriptor of redox chemistry. We found that while agglomeration lowers the NPs' surface areas, the interface-specific defects might lead to an activation of agglomerated NPs toward redox processes. Our results pave the way for an increased understanding of ceria NP agglomeration.

- [1] S. Schlick et al., J. Phys. Chem. C 120, 2016, page 6885
- [2] M. Lykaki et al, RSC Adv. 7, 2017, page 6160
- [3] G. Kresse and J. Furthmüller, Phys. Rev. B 54, 1996, page 11169
- [4] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 1996, page 3865
- [5] G. Kresse and D. Joubert, Phys. Rev. B 59, 1999, page 1758
- [6] S. L. Dudarev, et al., Phys. Rev. B 57, 1998, page 1505
- [7] M. Elstner et al., Phys. Rev. B 58, 1998, page 7260
- [8] B. Aradi, B. Hourahine, and T. Frauenheim, J. Phys. Chem. A 111, 2007, page 5678
- [9] J. Kullgren et al., J. Phys. Chem. C 121, 2017, page 4593
- [10] A. C. T. van Duin et al., J. Phys. Chem. A 105, 2001, page 9396
- [11] P. Broqvist et al., J. Phys. Chem. C 119, 2015, page 13598

---

## A2P2, Python Package for Automated Atomistic Simulations

P38

Chan-Woo Lee, Kanghoon Yim, Jehyun Lee, Byung Hyun Kim, Joonhee Kang<sup>\*</sup>

<sup>\*</sup> Platform Technology Laboratory, Korea Institute of Energy Research

We present our code, Automated Atomistic simulation management Platform in Python (A2P2) which we have been developing. Currently, the code consists of Interface atom extractor and Automatic molecule locator. The former can extract various kind of interfaces using advanced numerical algorithms. The latter specifically screen adsorption sites with similar local geometries, and can adsorb various molecules under diverse situations. We demonstrate how the code works, and how the code is applied to actual model interfaces. Finally, we share our visions to expand capabilities of A2P2 code.

[1]

---

## Predicting magnetic dilution effects in mononuclear single molecule magnets

P39

Leonel Llanos\* and Daniel Aravena\*  
\* *Universidad de Santiago de Chile*

The discovery of Single Molecule Magnets (SMM) has motivated the design and study of several molecular systems which exhibit slow magnetic relaxation with a wide range of blocking temperatures. Among the compounds which present slow magnetic relaxation there has been a significant leap on the performance of SMM behavior of lanthanide based complexes in the last years. Although the operative temperature of SMMs has reached a record (above liquid nitrogen temperature for some dysprosocenium derivatives) through ligand field design, there are other factors affecting the demagnetization phenomena. An experimentally accessible approach to improve SMM properties is reduction of spin-spin dipolar interactions through magnetic dilution, replacing paramagnetic ions for diamagnetic analogs. Hence, quantum tunneling is suppressed and demagnetization times are extended.

In this work, we present a general relation for the enhancement of relaxation time in SMMs upon magnetic dilution in a broad concentration range. Computational results are based on a recently developed model for the prediction of relaxation times in the tunneling regime. [1] The model is now extended to account for magnetic dilution. [2] The dependence of tunneling time with respect to dilution ratio was calculated for benchmark set of 18 mononuclear SMMs. All curves present a similar dependence both in shape and in order of magnitude, suggesting a general behavior for this phenomenon. This result is then rationalized in terms of a simple physical model considering the interaction of a single magnetic center with a variable number of magnetic neighbors. Finally, predictions are compared with experimental information for three cases, revealing a satisfactory agreement between experiment and theory.

[1] D. Aravena, *J. Phys. Chem. Lett.* 9 (2018) 5327 – 5333.

[2] L. Llanos, D. Aravena, Submitted.

## Phonon symmetry selection in intralayer and interlayer electron-phonon interactions in twisted bilayer graphene

P40

Eliel G. Silva Neto\*, M. V. O. Moutinho<sup>†</sup>, A. Righi<sup>‡</sup>, Po-Wen Chiu<sup>4</sup>, M. Paillet<sup>5</sup>, T. Michel<sup>5</sup>,  
M. A. Pimenta<sup>‡</sup> and P. Venezuela\*

\* *Instituto de Física, UFF, Brazil.*

<sup>†</sup> *NUMPEX-COMP, UFRJ, Brazil*

<sup>‡</sup> *Departamento de Física, UFMG, Brazil*

<sup>4</sup> *National Tsing Hua University, Hsinchu, Taiwan*

<sup>5</sup> *Laboratoire Charles Coulomb, CNRS, Univ. Montpellier, France*

Two-dimensional materials have attracted much attention in many fields of physics due to their electrical, magnetic, optical and mechanical properties. The possibility of combine those properties producing ultrathin devices is outstanding. Stacking those materials to create van der Waals heterostructures originates new physical phenomena. The possibility of a stack engineering in ultrathin van der Waals heterostructures comes with the challenge of understanding elemental excitations, such electrons, and phonons, in this scenario[1]. It is already known that the electron-phonon (el-ph) interactions in layered materials can occur involving electrons in the same layer (intralayer) or different layers (interlayer)[2]. Here we report the difference of the phonons activation via Raman spectroscopy for each process in twisted bilayer graphene samples. Our twisted bilayer graphene samples were produced via a chemical vapor deposition technique and then transferred to a fused silica substrate and present different stacking angles. The Raman spectroscopy results show the activation of optical and acoustic phonons in both processes. In the case of the interlayer process, all the folded phonon branches of the graphene can be observed in the Raman spectra when the laser energy is close to the energy difference between the van Hove singularities of the twisted bilayer graphene electronic structure. On the other hand, in the resonant intralayer process, only phonons that respect the symmetry selection rules of graphene along the  $\Gamma$  symmetry line can be measured via Raman spectroscopy for the analyzed angle range. Additionally, the high dispersion of the acoustic phonons concerning the sample angle can be useful for using Raman spectroscopy as an angle stacking measurement protocol for this system. DFT theoretical simulations for electrons and phonons gives support to the experiment. These results reinforce proposed intralayer/interlayer processes nomenclature for Raman signature graphene structures and may occur in other materials.

[1] Van der Waals heterostructures, A. K. Geim and I. V. Grigorieva, *Nature* v 499, p 419 – 425 (2013)

[2] Intralayer and interlayer electron-phonon interactions in twisted graphene heterostructures; G. S. N. Eliel et al; *Nature Communications* v 9, Article number: 1221 (2018)

## DFT study of novel 3D C60 polymers

P41

Jorge Diogo Marques Laranjeira\*

\* *CICECO-Aveiro Institute of materials*

New three-dimensional (3D) C60 polymerized structures, in which each molecule adopts either one of the two standard orientations, have been investigated using the density functional theory (DFT) method. Ordered binary-alloy type structures (AuCuI, , CuPt, “ ” ) were used as prototypes in constructing 3D C60 polymerized structures, one standard orientation corresponding to the A atom and the other orientation to the B atom. DFT structural optimizations show that intermolecular bonds, 56/56 2+2 cycloaddition, form between molecules with different orientations but no intermolecular covalent bond is formed between similarly oriented molecules, and, thus, the intermolecular covalent bonding can be mapped on to the antiferromagnetic interaction. This intermolecular bonding type forms between two intramolecular single bonds of neighbouring molecules and differs from the more common 66/66 2+2 cycloaddition that forms between intramolecular double bonds. The electronic and elastic properties of these polymerized structures were also calculated, within the general gradient approximation framework, at room pressure and at 9.5 GPa. All these structures show metallic behaviour [1] and their bulk moduli range from 88 to 132 GPa [2]. These 3D polymerized structures are likely to be prepared at 9.5 GPa and 550°C, although the observed fcc structure points to a disordered/frustrated structure, which is characteristic of the Ising antiferromagnetic interactions in the fcc lattice [3].

- 1 J. Laranjeira, L. Marques, N. Fortunato, M. Melle-Franco, K. Strutyński, M. Barroso, *Carbon* 137, (2018) 511-518.
- 2 J. Laranjeira, L. Marques, M. Melle-Franco, K. Strutyński (to be published).
- 3 J. Laranjeira, L. Marques, M. Mezouar, M. Melle-Franco, K. Strutyński, *Phys. Stat. Sol. RRL* 11 (2017) 1700343.

[1]

---

## Synergistic application of XPS and DFT to investigate Metal Oxide Surface Catalysis

P42

Quang Thang Trinh\*, Samir H. Mushrif† and Matthew P. Sherburne‡

\* *Cambridge Centre for Advanced Research and Education in Singapore (CARES), 1 Create Way, Singapore 138602, Singapore*

† *Department of Chemical and Materials Engineering, University of Alberta, 9211-116 St NW, Edmonton, Alberta T6G1H9, Canada*

‡ *Materials Science and Engineering Department, University of California, Berkeley, Berkeley, California 94720, United States*

Density Functional Theory (DFT), and experimental surface characterization techniques like X-ray Photoelectron Spectroscopy (XPS) are often used independently by computational and experimental researchers, respectively, to provide insights into metal oxide catalysed reaction mechanisms, pathways, and energetics. It is vital to develop novel approaches that integrate these surface sensitive experimental techniques and theoretical tools to gain better understanding of transition metal oxide (TMO) catalysed surface reactions. However, determining an appropriate Hubbard U-correction term is a challenge for the DFT community and identifying realistic reaction intermediates and their corresponding XPS shifts is a challenge for experimental researchers [1,2]. In this work, using CuO as a model TMO, we demonstrate an integrated experimental and theoretical approach to (i) determine the optimum U value range for TMOs, and, (ii) identify adsorbate/intermediate species on the TMO surface (and their XPS shifts), in a synergistic manner [1]. DFT+U is

used to calculate the Core-Level Binding Energy (CLBE) shifts for the possible adsorbed moieties, in various configurations, on both, clean and vacancy defect containing surfaces. We scan the theoretical CLBEs over a range of U values and compare the experimental and theoretical CLBEs of the aforementioned adsorbates, to provide an appropriate U value that predicts the experimental shifts correctly. In the process of U value determination, we parallelly uncover the existing surface moieties, their adsorption configurations and their XPS shifts. The U value between 4-5 eV correctly establishes the experimental XPS peaks to the respective adsorbates and their geometries. This U value differs significantly from the bulk properties fitted U value of 7 eV and is in excellent agreement with our recent DFT+U benchmarking study based on the heat of adsorption and Fourier Transform Infrared Spectroscopy measurements [3]. The method demonstrated in this paper can be extended to other TMOs, as well as to advanced surface characterization methods like temperature programmed XPS and in situ XPS studies to gain mechanistic insights into complex reactions and to guide the design and development of efficient and novel TMO based catalysts.

- [1] Trinh et al., J. Phys. Chem. C 2018, 122, 22397-22406.
- [2] Capdevila-Cortada et al., ACS Catal. 2016, 6, 8370-8379.
- [3] Bholal et al., J. Phys. Chem. C 2017, 121, 21343-21353.

---

## Ligand engineering in Cu(II) paddle wheel metal-organic frameworks for enhanced electrical conductivity

P43

Matthias Golomb\*, Joaquin Calbo\* and Aron Walsh\*  
\* *Imperial College London*

In recent years, engineering electrically conductive metal-organic frameworks (MOFs) has become of interest due to their potential application in new application areas including batteries and supercapacitors[1]. However, most of these materials exhibit a very localized charge carrier (electron and hole) density and are thus very poor conductors. There exist multiple approaches to enhance conductivity in MOFs, such as the introduction of guest molecules[2] or mixed valency[3]. In this study, we calculated the electrical properties of MOFs based on copper paddle wheels. This structure offers local metal-metal electronic mobility, and we chose to combine it with the ligand diazabicyclooctane (dabco) due to a possibly good band alignment and spatial overlap of the nitrogen p-electrons with the copper d-electrons. MOF- 649 shows no significant dispersion and charge carrier mobility for the HOMO and LUMO states, whereas DMOF-1 exhibits the desired features. The aim is to further establish a set of design criteria for controlling electronic overlap between the organic and inorganic components of hybrid framework materials.

- [1] Wang, L. et al, 2016, Coordination Chemistry Reviews 307, 361 – 381
- [2] Talin, A.A. et al, Science 343, 66 – 69
- [3] Xie, L.S. et al, 2018 Journal of the American Chemical Society 140, 7411 – 7414

---

## Stabilizing Potential Superalloys

P44

Tyler Whitaker\*

\* *Brigham Young University*

Superalloys are materials that have very useful properties, including things like superior mechanical properties, and better high temperature performance. A search for novel materials is always underway in an effort to maximize effectiveness of our tools. Computational methods have been developed to expedite that search by using Density Functional Theory from Quantum Mechanics to model materials that have never been created before. A set of proposed superalloys [1] was found to be metastable [2], causing the desired properties to be lost after some time. This project explores the possibility of adding additional elements to the aforementioned alloys in an effort to stabilize the superalloy phase. This presentation explores the methods that will be used to model the alloys with the additional elements.

[1] Nyshadham et al., *Acta Materialia*, Volume 122, 1 January 2017, Pages 438-447

[2] F. L. R. Tirado, J. P. Toinin, and D. C. Dunand, *Acta Materialia*, Volume 151, 1 June 2018, Pages 137-148

---

## Electronic and vibrational properties of Copper Indium Selenide: Impact of hybrid functionals on phonons

P45

Sandeep Kumar\* and Ludger Wirtz\*

\* *Physics and Materials Science Research Unit, University of Luxembourg, 1511 Luxembourg, Luxembourg*

We have performed first-principles calculations of the electronic structure and the lattice dynamics of  $CuInSe_2$  both in the chalcopyrite structure and with Cu-Au ordering of the cation sublattice. We have used density functional theory (DFT), as implemented in the Vienna Ab initio Simulation Package (VASP) and CRYSTAL code. Since the semi-local PBE and LDA functionals lead to a closure of the gap for both phases of  $CuInSe_2$ , we investigate – via the use of the hybrid functional - the effect of Hartree-Fock exchange on the band-structure and the resulting phonon frequencies. The calculated Raman and infrared active phonon frequencies are in reasonable agreement with the experimental values and other calculations.

[1]

---

## Investigations of order-disorder phase transitions in high entropy alloys with the use of machine-learning interatomic potentials

P46

Tatiana Kostiuchenko\*, Alexander Shapeev\*, Fritz Körmann<sup>†,‡</sup> and Jörg Neugebauer<sup>†</sup>

\* *Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Nobel St. 3, Moscow, 143026, Russia*

<sup>†</sup> *Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany*

<sup>‡</sup> *Materials Science and Engineering, Delft University of Technology, 2628 CD Delft, The Netherlands*

High-entropy alloys (HEA) is a class of materials that have high ductility and yield strengthening, they are widely used as construction and heat-resistant materials. HEAs consist of at least four different chemical elements and have a specific structure, because of different sizes and electrochemical properties of elements.

Experimental methods of HEAs investigation are time-consuming, they give a poor representation of structure specifics at low temperatures. Thus computational methods of HEAs investigation are of the high interest in materials design. In this work, a new methodology is proposed to investigate the stability of the solid solution phase in HEAs. It includes the machine-learning “on-lattice” model used as an atomic interaction model in canonical Monte Carlo to investigate the stability of HEAs.

This interaction model, namely low-rank potential (LRP) [1], is a data-driven method and requires a training set, that consists of small configurations with their reference energies. In the proposed approach we use calculations based on density functional theory (DFT) to obtain these reference energies. LRP that was trained on relatively big training set with accurate data is able to predict the energy of systems with high accuracy. Moreover, adding new configurations to the training set from Monte Carlo calculations proceeded helps to increase the accuracy of LRP predictions, so the prediction error comes to 1 meV/atom.

We examined our approach in comparison with recent work [2] and then on the example of NbMoTaW equiatomic system we demonstrated the importance of account for local lattice distortions. It was shown that solid solution in NbMoTaW stays stable till room temperatures. The mechanisms of chemical ordering were also investigated in this work.

[1] Shapeev A., *Computational Materials Science* 139, 26 – 30, 2017

[2] Körmann F., Ruban A. V. & Sluiter M. H., *Materials Research Letters* 5, 35 – 40, 2017

---

## Graph similarity drives zeolite diffusionless transformations and intergrowth

P47

Daniel Schwalbe-Koda\* and Rafael Gómez-Bombarelli\*

\* *Massachusetts Institute of Technology, Department of Materials Science and Engineering*

Zeolites are inorganic nanoporous materials with broad applications as selective catalysts, ion exchangers, and separators. Despite sustained research, directing polymorphic transformations is still a critical challenge in zeolite design, relying mostly on trial-and-error. Ab initio calculations could guide the synthesis of new frameworks, but the combinatorial number of theoretically accessible zeolites render this approach computationally prohibitive. Complex crystallization mechanisms further hinder the theoretical modeling. In our studies, we combine big-data, natural-language processing, crystallography, graph theory, and structural kernels to explain phase transformations in zeolites and screen promising topologies for catalytic applications.

Within a corpus of more than 70,000 articles on zeolites, 374 reports of zeolite polymorphic relations are found. The data suggests that traditional structure descriptors are weak predictors of topology interconversion and insufficient to explain intergrowth. By introducing a supercell-invariant metric that compares crystal structures using graph theory, we show that topotactic and reconstructive (diffusionless) transformations occur only between topologically-similar pairs. Furthermore, all known instances of intergrowth take place between either structurally-similar or graph-similar frameworks. Supported by exhaustive literature results, we single out promising pairs for realizing novel diffusionless transformations and intergrown composite zeolites. Hundreds of low-distance pairs are identified among known topologies, and thousands of hypothetical frameworks are associated to known zeolites counterparts. These insights suggest novel frameworks to be further investigated through density functional theory calculations and coupled to chemical reactions through molecular dynamics simulations, reactive force fields, and high-throughput virtual screening. This integrated theoretical pipeline opens a venue to zeolite discovery and understanding.

- [1] D. Schwalbe-Koda et al. Graph similarity drives zeolite diffusionless transformations and intergrowth. Under review, 2019.

---

## Phenylated Acene Derivatives as Candidates for Intermolecular Singlet Fission

P48

Xiaopeng Wang\*, Xingyu (Alfred) Liu\*, Rithwik Tom\*, Cameron Cook†, Bohdan Schatschneider†  
and Noa Marom\*

\* *Carnegie Mellon University*

† *California State Polytechnic University at Pomona*

Singlet fission (SF), a spin-conserving process where one singlet exciton is converted into two triplet excitons, may improve the efficiency of organic photovoltaics. Only a few materials have been experimentally observed to undergo intermolecular SF, most of which are acenes and their derivatives. Using many-body perturbation theory in the GW approximation and the Bethe – Salpeter equation, we systematically investigate the electronic and excitonic properties of tetracene, pentacene, and their phenylated derivatives in the gas phase and solid state. Their potential for SF is evaluated with respect to the thermodynamic driving force and the singlet exciton charge-transfer character. In both the gas phase and solid state, pentacene and its derivatives are more promising than tetracene analogues. Within a family of molecules containing the same acene backbone, increasing the number of phenyl side groups is detrimental for the SF driving force in the gas phase.



However, in the solid state, the SF driving force and the exciton character are modulated by intermolecular interactions present within different packing arrangements. Molecules with a higher number of phenyl side groups often form crystals with less cofacial interactions between the acene backbones. These crystals are found to exhibit a higher SF driving force and a higher degree of singlet exciton charge-transfer character. In particular, 5,7,12,14-tetraphenylpentacene, 1,4,6,8,11,13-hexaphenylpentacene, and 1,2,3,4,6,8,9,10,11,13-decaphenylpentacene emerge as promising candidates for intermolecular SF in the solid state.

[1] Wang et al., J. Phys. Chem. C 2019, 123, 5890 – 5899

---

## Tuning TCNQ adsorption on Ag(100): A joint DFT and experimental study of the role of alkali co-adsorption

P49

Billal Sohail\*, Luke Rochford<sup>†</sup>, Phil blowey<sup>\*,‡</sup>, Phil Woodruff<sup>4</sup>, Giovanni Constantini\* and Reinhard Maurer\*

\* *Department of Chemistry, University of Warwick, UK*

<sup>†</sup> *School of Chemistry, University of Birmingham, UK*

<sup>‡</sup> *Diamond Light Source, Didcot, OX110DE, UK*

<sup>4</sup> *Department of Physics, University of Warwick, UK*

TCNQ(7,7,8,8-tetracyanoquinodimethane) is a well-established electron acceptor with an innate ability to form conductive organic salts. The application of organic semiconductors on coinage metals is a growing field which lends to the understanding of molecular electronics. A multidisciplinary field which has piqued in recent years due to the variety of applications such as, organic photovoltaics (OPVs), organic field effect transistors (OFETs). TCNQ alone on coinage metal surfaces conforms to a specific geometry with the peripheral cyano groups bent towards the surface; an effect lifted upon co-adsorption with potassium. The work presented is to elucidate the underlying mechanism of charge transfer and dispersion interactions using theoretical and computational efforts. Combining many-body-dispersion-inclusive Density-Functional Theory [1] and experimental techniques such as X-ray standing wave (XSW) data and STM measurements.

1 Maurer et al., J. Chem. Phys., 143, 102808 (2015)

---

## Reaction Mechanisms of the High Temperature Oxygen Evolution Reaction

P50

Hanna Tuerk\*, Christoph Scheurer\* and Karsten Reuter\*

\* *Technical University of Munich*

The climate-induced demand for global decarbonization evoked a search for alternative energy carriers. A promising candidate is hydrogen, due to its sustainability and its extensive application possibilities as e.g. chemical reactant, energy storage and production of electricity in fuel cells [1].

A common way to produce hydrogen from water is in an electrolyzer under consumption of water and energy. Under the various existing types of electrolyzers, the highest Faradaic efficiencies are yielded by high temperature realizations such as solid oxide electrolysis cells (SOECs), due to the higher ionic conductivity in the electrolyte, the faster electrode reaction kinetics and the lower reaction over potentials at elevated temperatures [2].

However, SOECs are not yet ready to be commercialized, as their performance and lifetime are restricted due to degeneration of the cells anode [3]. In order to understand this limitation, this study investigates the microscopic cell processes by means of density functional theory. Two leading anode materials, lanthanum strontium manganite and lanthanum strontium cobaltite, are modeled on the standard electrolyte support yttria stabilized zirconia to capture the whole triple phase boundary, where the reaction takes place. Thus, the mechanism of the oxygen evolution reaction and the electrodes degeneration can be clarified. The gained knowledge will be employed to develop electrode design strategies in order to enhance cell performance.

- [1] Foit, S. R.; Vinke, I. C.; Haart, L. G. J. D.; Eichel, R. *Angew. Chem. Int. Ed.* **2017**, *56*, 5402.
- [2] Hauch, A.; Ebbesen, S. D.; Jensen, S. H.; Mogensen, M. *J. Mater. Chem.* **2008**, *18*, 2331.
- [3] Sohal, M. S.; O'Brien, J. E.; Stoots, C. N.; Sharma, V. I.; Yildiz, B.; Virkar, A. *J. Fuel Cell Sci. Tech.* **2012**, *9*, 011017.

---

## DFT based screening for oxide supported catalyst materials

P51

Frederic Felsen\*, Christoph Scheurer\* and Karsten Reuter\*

\* *Technical University of Munich*

Methanol production via catalytic hydrogenation of carbon dioxide attracts both industrial and environmental interest. Methanol is an essential building block in the synthesis of higher alkanes and alcohols. Developing novel catalyst materials is an opportunity to satisfy the steadily increasing demand for methanol while simultaneously facing the growing atmospheric carbon dioxide concentration. Computational screening methods may provide a promising pathway for exploring the vast space of potential catalyst materials for this process. To date, corresponding studies are typically performed for the (presumably) active material itself, e.g. transition metal (TM) or TM alloy catalysts [1,2]. This might not appropriately address the well-known subtleties in geometric and electronic structure of multi-component heterogeneous catalysts, like the state-of-the-art Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> catalyst for industrial CO<sub>2</sub> hydrogenation [3]. In our work we aim to tackle this challenge by establishing an extended DFT data base of model systems that suitably mimic such multi-component systems. We then plan to establish refined screening models on the basis of this data that then allow for a first assessment of the degree to which existing knowledge from active-material-only screening studies needs to be adapted.

- [1] F. Studt, F. Abild-Pedersen, Q. Wu, A. D. Jensen, B. Temel, J.-D. Grunwaldt, J. K. Nørskov, *J. Catal.*, 293, (2012).
- [2] F. Studt, I. Sharafutdinov, F. Abild-Pedersen, C. Elkjær, J.S Hummelshøj, S. Dahl, I. Chorkendorff, J. K. Nørskov, *Nat. Chem.*, 320, (2014).

- [3] M. Behrens, F. Studt, I Kasatkin, S. Kühn, M. Hävecker, F. Abild-Pedersen, S. Zander, F. Girgsdies, P. Kurr, B. L. Kniep, M. Tovar, R. W. Fischer, J. K. Nørskov, R. Schlögl, *Science*, 336, (2012).

---

## All-Zinc Coordinated Nickel-Complexes as Molecular Mimics for NiZn Catalyst Surfaces, a Density Functional Theory Study

P52

Julius Hornung\*, Maximilian Muhr\*, Christian Gemel\* and Roland A. Fischer\*

\* *Chair of Inorganic and Metal-Organic Chemistry, Technical University of Munich, Lichtenbergstr. 4, 85748 Garching, Germany. E-mail: roland.fischer@tum.de*

A perspective connection between Hume-Rothery inspired TM/E (TM = transition metal; E = Al, Ga, Zn) complexes and clusters [1] with the related solid-state intermetallic TM/E compounds is presented with respect to the industrially relevant catalytic semihydrogenation of acetylene.[2] The theoretical study dealing with  $[\text{Ni}(\text{ER})_n(\text{C}_2\text{H}_x)_{4-n}]$  ( $x = 2, 4$ ;  $\text{R} = \text{CH}_3, \text{C}_5\text{Me}_5$ ) calculated on the DFT level of theory shows intriguing structural and electronic properties of the examined complexes. Different Ni-E complexes show preferred binding of  $\text{C}_2\text{H}_2$  over  $\text{C}_2\text{H}_4$  in bridging positions between Ni and E depending on the  $[\text{Ni}(\text{ER})_n]$  fragment. These findings render molecular TM/E systems, such as Ni/Zn, promising candidates to mimic key intermediates of intermetallic catalysts applied in heterogeneous hydrogenation reactions. We put these findings into the context of existing synthetic results and illustrate different experimental approaches to obtain compounds of the general formula  $[\text{TM}_a\text{E}_b](\text{Cp}^*)_c(\text{UHC})_d$  (UHC = unsaturated hydrocarbon ligands) as potential surface models.

[1] Mayer, K.; Weßing, J.; Fässler, T. F.; Fischer, R. A., *Angew. Chem. Int. Ed.* 2018, 57, 14372.

[2] Studt, F.; Abild-Pedersen, F.; Bligaard, T.; Sørensen, R. Z.; Christensen, C. H.; Nørskov, J. K., *Science* 2008, 320 (5881), 1320-1322.

---

## The Role of Charge Transfer in the $\text{CO}_2$ Activation on $3d \text{ TM}_{13}$ Clusters: A DFT Investigation

P53

Vivianne K. Ocampo-Restrepo\*, Larissa Zibordi-Besse\* and Juarez L. F. Da Silva\*

\* *São Carlos Institute of Chemistry, University of São Paulo, PO Box 780, 13560 -970, São Carlos, SP, Brazil.*

Decreasing the concentration of  $\text{CO}_2$  in the atmosphere is essential to mitigate the impact of global warming.<sup>1</sup> For that, one of the promising strategies is to convert  $\text{CO}_2$  into higher value products through reduction; however, activating this molecule is difficult and also the conversion processes tend to be slow, being necessary the use of catalysts.<sup>1</sup> In this sense, from the computational point of

view and using the Fritz-Haber *ab initio* molecular simulations package, this work provide insights of how CO<sub>2</sub> interacts and activates on 3d TM<sub>13</sub> clusters.<sup>2</sup>

The magnitude of the adsorption energy,  $E_{ad}$ , indicates that the adsorption strength of CO<sub>2</sub> on the TM<sub>13</sub> clusters follows a periodic trend. In accordance to that, the C–O bond and OCO angle compared to CO<sub>2</sub> gas phase presented, respectively, an increase around 6.84–7.70% and a decrease around 22.96–24.32% for Fe<sub>13</sub>, Co<sub>13</sub>, and Ni<sub>13</sub>, while there were negligible structural modifications in the molecule for CO<sub>2</sub>/Cu<sub>13</sub>. Thus, as stronger as  $E_{ad}$ , higher is the geometric variations on the CO<sub>2</sub>, and vice-versa. Besides, the adsorption site preference in the lowest energy structure revealed that the CO<sub>2</sub> was coordinated in a bridge site on Fe<sub>13</sub>, Co<sub>13</sub>, and Ni<sub>13</sub> clusters, and in a top site on Cu<sub>13</sub> cluster. Hence, the molecule coordination is associated with its structural modifications, which permit to evaluate the activation of the molecule.

Also, to understand the character of the interaction between the molecule and the TM<sub>13</sub> clusters, we calculated the net charge at the molecule after the adsorption,  $\Delta q_{CO_2}$ . The results show that the CO<sub>2</sub> present a partial negative charge when adsorbs on Fe<sub>13</sub>, Co<sub>13</sub>, and Ni<sub>13</sub>, indicating that those clusters donate charge to the molecule and, on the other hand, the  $\Delta q_{CO_2}$  on Ni<sub>13</sub> was found as almost zero. Furthermore,  $\Delta q_{CO_2}$  evaluates the grade of perturbation at CO<sub>2</sub> due to the adsorption, within those results being consistent with the  $E_{ad}$  and the CO<sub>2</sub> structural modifications, which allow us to classify the interaction as chemical adsorption on Fe<sub>13</sub>, Co<sub>13</sub>, and Ni<sub>13</sub>, and physical adsorption on Cu<sub>13</sub>, revealing the role of TM in the adsorption. Hence, the Fe<sub>13</sub>, Co<sub>13</sub>, and Ni<sub>13</sub> clusters promote the activation of CO<sub>2</sub> by the chemisorption, and the Cu<sub>13</sub> cluster favors its physical adsorption.<sup>2</sup>

[1] Esrafilzadeh, D.; Zavabeti, A.; *et al. Nat. Commun.*, **2019**, 10(865), 1 – 8.

[2] Ocampo-Restrepo, V. K.; Zibordi-Besse, L.; Da Silva, J. L. F. DFT Investigation of CO<sub>2</sub> Adsorption on 3d TM<sub>13</sub> Clusters. Manuscript in preparation.

---

## ***Ab initio* Investigation of Mixture of CeO<sub>2</sub>-ZrO<sub>2</sub> Nanoclusters and Adsorption of Zr-adatoms on the CeO<sub>2</sub> (111) Surface**

P54

Priscilla Felício-Sousa\*, Johnatan Mucelini\*, Larissa Zibordi-Besse\*, Karla F. Andriani\*,  
Rafael Costa-Amaral\* and Juarez L. F. Da Silva\*

\* São Carlos Institute of Chemistry, University of São Paulo, São Carlos, Brazil.

The mixing of ceria and zirconia have been considered as promising candidates for the conversion of methane into high-value products, i.e., methanol, dimethyl ether, etc. The most import figures of merit of ceria-zirconia catalysts are based on the oxygen storage capacity, which can be partially explained by the ability of cerium atoms to exchange the oxidation state. Thus, there is a great interest to understand the mixing of ceria-zirconia at the nanoscale, as well as the formation of ZrO<sub>2</sub>-like films on the CeO<sub>2</sub> (111) surface. In this context, for this study we performed an *ab initio* Density Functional Theory and DFT+U investigation, at PBE level (HSE06 - nanoclusters putative global minimum configurations) as well as post-statistical analysis to establish relationships between the structural and electronic characteristics with the nanoclusters energy-formation. We found that Zr atoms have a strong preference for the core region of the cluster, which can be

explained by the different cations radii, i.e., the smaller Zr radius helps to release the strain energy. We found negative formation energy ( $T = 0K$ ) values for the ceria-zirconia nanoclusters, which indicates an energetic preference for mixing. The lowest formation energy (high stability) was obtained for  $x = 0.27$ , within close agreement with experimental observations. For Zr/CeO<sub>2</sub> (111), we found a strong preference of Zr adatoms to the O<sup>2-</sup> anions sites, which can be explained by the strong Coulomb interactions, and for every Zr adatom on the surface, 4 Ce atoms change the oxidation state from +IV to +III, which induces the creation a large strain within the topmost ceria surface layers. Thus, the surface undergoes strong reconstructions to release the strain energy, which favors the formation of the ZrO<sub>2</sub>-like layers on the ceria surface. Our findings are consistent with experimental observations, which was obtained by scanning tunneling microscopy. This study was financed in part by the CAPES - Finance Code 001, CNPq, and also supported by FAPESP, project N°. 2018/11152-0.

- [1] Felício-Sousa P., et al., Manuscript in process.
- [2] Mucelini J., et al. Chem. Phys. 2018, 149, 244702-(1 to 8);
- [3] Zibordi-Besse L., et al., J. Phys. Chem. C, 2018, 122 (48), 7702-27712.
- [4] Piotrowski, M. J., et al., J. Phys. Chem. C, 2014, 188 , 21438 – 21446.

---

## Bandgap and pseudohelicity effects over conductance in gapped graphene junctures

P55

Jorge Andres Navarro-Giraldo<sup>\*,†</sup> and Carlos Quimbay<sup>‡</sup>

<sup>\*</sup> CEITEC - Central European Institute of Technology, Brno, Czech Republic

<sup>†</sup> Brno University of Technology, Brno, Czech Republic

<sup>‡</sup> Universidad Nacional de Colombia, Bogota D.C., Colombia

We study the conductance in gapped single-layer graphene junctures as a function of the bandgap, pseudohelicity and charge carrier density. To this end, we first calculate the transmission coefficients for helicity-polarized massive charge carriers on p – n and n – p – n junctures of gapped single-layer graphene. Next, we calculate the conductance for these two systems using the Landauer formula. For the p – n juncture case, we find the existence of a contribution to the conductance from pseudohelicity inversion states, which is dominant in p-n or n-p junctures, compared to the contribution from pseudohelicity conservation states. In the n-p-n juncture, the conductance is entirely through helicity conserved states. Also, we find for both type of junctures that there exists a window of charge carriers densities values where the conductance is zero (conductance gap), such that the size of this window depends on the bandgap squared. We observe that the existence of a bandgap in the system leads to valley mixing, a fact that could be useful in the design of devices based on single-layer gapped graphene.

Our results were published in reference [1].

- [1] J A Navarro-Giraldo and C J Quimbay 2018 J. Phys.: Condens. Matter **30** 265304  
<https://doi.org/10.1088/1361-648X/aac61f>

---

## The dynamic structure factor of warm dense copper

P56

Maximilian Schörner\*

\* *University of Rostock*

Ab initio simulations using density functional theory combined with molecular dynamics allow for a self-consistent description of copper in the warm dense matter regime, which is characterized by strong correlation and degeneracy effects. The inner dynamics of the system can be described by the dynamic structure factor of the electrons and ions which is accessible in the simulations. These quantities are also closely connected to material properties like the speed of sound and the dynamic electrical conductivity and can be measured directly in inelastic scattering experiments[1].

This work establishes good agreement of simulation results with experimental data for copper under ambient pressure in the liquid and heated solid phase. Material properties like compressibility, speed of sound and dynamic electrical conductivity can also be extracted. The investigation is extended to the warm dense matter regime where the used approach has previously produced good results for aluminum [2] and lithium [3]. The dynamic ion structure factor of copper is computed at temperature in excess of 1 eV and solid state densities. Experimentally, these conditions have become accessible in shock compression experiments, which will allow a verification of the obtained simulation results. If successful, this approach could serve as a blue print for describing mid to high Z elements similar to copper.

[1] S. H. Glenzer and R. Redmer, *Rev. Mod. Phys.* 81, 1625 (2009)

[2] H. R. Rüter and R. Redmer, *Phys. Rev. Lett.* 112, 145007 (2014)

[3] B. B. L. Witte, M. Shihab, S. H. Glenzer, and R. Redmer, *Phys. Rev. B* 95, 144105 (2017)

---

## Ab initio molecular dynamics simulations of negative thermal expansion in ScF<sub>3</sub>: the effect of the supercell size

P57

Dmitry Bocharov\*, Matthias Krack†, Yuri Rafalskij\*, Alexei Kuzmin\* and Juris Purans\*

\* *Institute of Solid State Physics, University of Latvia, Kengaraga street 8, LV-1063 Riga, Latvia*† *Paul Scherrer Institute, Forschungsstrasse 111, CH-5232 Villigen PSI, Switzerland*

Scandium fluoride (ScF<sub>3</sub>) belongs to a class of negative thermal expansion (NTE) materials. It shows a strong lattice contraction up to about 1000 K switching to expansion at higher temperatures. Here the NTE effect in ScF<sub>3</sub> is studied in the temperature range from 300 K to 1600 K using ab initio molecular dynamics (AIMD) simulations in the isothermal-isobaric (NpT) ensemble. The temperature dependence of the lattice constant, inter-atomic Sc–F–Sc bond angle distributions and the Sc–F and Sc–Sc radial distribution functions is obtained as a function of supercell size from  $2a \times 2a \times 2a$  to  $5a \times 5a \times 5a$  where  $a$  is the lattice parameter of ScF<sub>3</sub>. A comparison with the experimental Sc K-edge EXAFS data at 600 K is used to validate the accuracy of the AIMD simulations. Our results suggest that the AIMD calculations are able to reproduce qualitatively the NTE effect in ScF<sub>3</sub>, however a supercell size larger than  $2a \times 2a \times 2a$  should be used to account accurately for

dynamic disorder. The origin of the NTE in  $\text{ScF}_3$  is explained by the interplay between expansion and rotation of  $\text{ScF}_6$  octahedra.

The calculations were performed on the Paul Scherrer Institute cluster Merlin4, HPC resources of the Swiss National Supercomputing Centre (CSCS) in Lugano (Project ID s628) as well as at the Latvian SuperCluster (LASC). The authors sincerely thank S. Ali, A. Kalinko, and F. Rocca for providing experimental EXAFS data, as well as M. Isupova, V. Kashcheyevs, and A. I. Popov for stimulating discussions. Financial support provided by project No. 1.1.1.2/VIAA/1/16/147 (1.1.1.2/16/I/001) under the activity “Post-doctoral research aid” is greatly acknowledged by D.B. A.K and J.P. would like to thank the support of the Latvian Council of Science project no. lzp-2018/2-0353.

- [1] B. K. Greve, K. L. Martin, P. L. Lee, P. J. Chupas, K. W. Chapman, A. P. Wilkinson, Pronounced negative thermal expansion from a simple structure: cubic  $\text{ScF}_3$ , *J. Am. Chem. Soc.* 132 (2010) 15496-15498.
- [2] D. Bocharov, M. Krack, A. Kalinko, J. Purans, F. Rocca, S. E. Ali, A. Kuzmin, Ab initio molecular dynamics simulations of the Sc K-edge EXAFS of scandium trifluoride, *J. Phys.: Conf. Ser.* 712 (2016) 012009.
- [3] D. Bocharov, M. Krack, J. Rafalskij, A. Kuzmin, J. Purans, Ab initio molecular dynamics simulations of negative thermal expansion in  $\text{ScF}_3$ : the effect of the supercell size, *Comp. Mat. Sci.* (2019) accepted.

---

## Experimental and theoretical study of nanoshaped Ni/CeO<sub>2</sub> catalysts for hydrogen production

P58

P. Pérez-Bailac\*, P. Lustemberg<sup>†</sup>, J. Vecchiotti<sup>†</sup>, L. Pascual\*, A. Martínez-Arias\*, A. Bonivardi<sup>‡</sup>  
and M. Verónica Ganduglia-Pirovano\*

\* *Institute of Catalysis and Petrochemistry-CSIC, Madrid, Spain*

<sup>†</sup> *Instituto de Física Rosario (IFIR), CONICET-UNR, Bv. 27 de Febrero 210 bis, S2000 EZP  
Rosario, Santa Fe, Argentina.*

<sup>‡</sup> *Instituto de Desarrollo Tecnológico para la Industria Química, UNL-CONICET, 3000 Santa Fe,  
Argentina*

Hydrogen is thought to be the solution as a clean and renewable future energy vector of the post petroleum era. It is possible to produce the hydrogen from the steam reforming of ethanol (ESR) [1]:  $\text{CH}_3\text{CH}_2\text{OH} + 3\text{H}_2\text{O} \rightarrow 2\text{CO}_2 + 6\text{H}_2$ , using Ni/CeO<sub>2</sub> catalysts. The activity of such catalysts mostly depends on the ceria facet exposed, metal loading, and metal-ceria interactions. Although the role of many of these factors is still unclear, and a generally accepted mechanism for the reaction does not yet exist. Real supported catalyst powders are very complex systems and a fundamental understanding of the above mentioned factors affecting catalytic activity is important for elucidating how these catalysts work.

In order to investigate the effect that the exposure of a specific termination has on the surface chemistry and catalytic activity, Ni stabilized by well-defined CeO<sub>2</sub> nanoshapes with distinct surface atomic arrangements, such as cubes [(100)], rods [(110) and (100)], spheres [(111) and (100)], and octahedral [(111)], have been synthesized [2] and characterized. It is observed that the catalytic activity does depend on the exposed surface facet of the ceria support.

With this in mind, and in order to gain a microscopic understanding of the effect that the exposure of a specific termination has on the surface chemistry and catalytic activity, theoretical models will be created and studied applying the spin-polarized density functional theory+U (DFT+U) approach, including van der Waals interactions, and in combination with statistical thermodynamics and transition state search methods. As a first step the interaction of the dissociative adsorption of ethanol on differently oriented CeO<sub>2</sub> surfaces in combination with IR spectroscopy is currently being considered; the exposed ceria facet is known to influence the chemisorption properties [3]. Next, the interaction of Ni nanoparticles with those surfaces will be addressed; metal-support interactions are likely to have an essential role in the systems' catalytic properties, as recently shown for the direct conversion of CH<sub>4</sub> to CH<sub>3</sub>OH over Ni/CeO<sub>2</sub> (111) [4]. Finally, the reaction mechanism that include elucidating the nature of active sites will be investigated for the most promising model catalysts. The synergy between theory and experimental work will be crucial to unravel the structure of the working catalysts while bridging the gaps between model and real powder catalysts.

- [1] T. Hou, et al. *Renew. Sust. Energ. Rev.* 44 (2015) 132-148.
- [2] J. Han, et al. *J. Mol. Catal. A Chem.* 335 (2011) 82-88.
- [3] Schilling, et al. *J. Phys. Chem. Lett.* 9 (2018) 6593 – 6598.
- [4] P. G. Lustemberg, et al. *J. Am. Chem. Soc.* 140 (2018) 7681 – 7687

---

## Exact-exchange effects in hybrid exchange-correlation functionals to describe metal oxides

P59

Marcos Rivera-Almazo\* and Jorge Garza\*

\* *Universidad Autonoma Metropolitana*

Oxides of transition metals and metalloids have been extensively studied from experimental and theoretical techniques since these systems exhibit unique properties, mainly linked to the strong correlation between their valence electrons. For computational studies, this electron correlation yields problems to reproduce both structural and electronic properties[1]. Within the Density Functional Theory in the Kohn-Sham formulation, exchange-correlation functionals with a contribution of exact exchange, such as PBE0 or B3LYP, improve the description of metal oxides. However, in multiple cases these approximations are not good to give a good description.

In this work we study one-parameter hybrid exchange-correlation functionals over MnO, SiO<sub>2</sub>, GeO<sub>2</sub>, SnO<sub>2</sub>, and ZrO<sub>2</sub>. The calculations were performed using a periodic ab initio code based on Gaussian localized basis functions for the expansion of Bloch orbitals by linear combination of atomic orbitals[2]. It is worth noting that by adjusting the fraction of the exact exchange in these hybrid functionals to reproduce the band gap, we found that in most of the studied cases we also reproduced other properties such as geometrical parameters and bulk moduli [3].

- [1] Singh H, Singh M, Kumar S, Kashyap MK (2011) Full potential calculation of electronic properties of rutile RO<sub>2</sub> (R=Si, Ge, Sn and Pb) compounds via modified Becke Johnson potential. *Phys B Condens Matter* 406:3825 – 3830
- [2] Dovesi R, Orlando R, Erba A, Zicovich-Wilson CM et al (2014) Crystal14: a program for the ab initio investigation of crystalline solids. *Int J Quantum Chem* 114:1287 – 1317



- [3] Alejandra M. Navarrete-López, Marcos Rivera-Almazo, Jorge Garza, Rubicelia Vargas. Importance of one-parameter hybrid exchange- correlation functionals in band gaps of transition metal and metalloid oxides (2018) *Theor. Chem. Acc.* 137, 36

## Sites for CO dissociation over platinum

P60

Noemi Bosio and Henrik Grönbeck\*

\* *Department of Physics and Competence Centre for Catalysis, Chalmers University of Technology, Sweden*

For decades there has been experimental indications of CO dissociation on different Pt surfaces [1-5]. The dissociation appears to depend sensitively on the surface structures. When operating at high pressure, dissociation was reported at 500 K for Pt(100), whereas a temperature of 673 K was required for dissociation on Pt(111) [5]. The dissociation was in Ref. [5] associated with a roughening of the surface via the formation of platinum carbonyls. The subject is puzzling, in part due to the lack of theoretical results to support the experimental observations. However, most computational studies have been carried out on flat surfaces where the reaction is very endothermic [6, 7].

In this study, CO dissociation has been investigated by density functional theory (DFT) using the Vienna Ab Initio Simulation Package (VASP). The generalized gradient approximation functional PBE was used to describe exchange-correlation effects. The Kohn-Sham orbitals were expanded in plane waves and the core-valence interactions was described within the plane augmented wave (PAW) method. Different sites for CO dissociation were investigated by considering different surfaces and sites including platinum carbonyls.

In accordance with previous studies, we find that direct dissociation from a low coverage state is highly activated and endothermic on flat surfaces such as Pt(111) and Pt(100) and also on stepped surfaces such as Pt(211). However, dissociation appears possible at special sites at high CO coverage.

- [1] Y.O. Park, R.I. Masel, K. Stolt, *Surf. Sci.* 131, L385-L389 (1983)
- [2] Y.O. Park, W.F. Banholzer, R.I. Masel, *Appl. Surf. Sci.* 19, 145 (1984)
- [3] Y.O. Park, W.F. Banholzer, R.I. Masel, *Surf. Sci.* 155, 341 (1985)
- [4] W.F. Banholzer, R.E. Parise, R.I. Masel, *Surf. Sci.* 155, 653 (1985)
- [5] K. R. McCrea, J. S. Parker, G. A. Somorjai, *J. Phys. Chem. B* 106, 10854 (2002)
- [6] Y. Morikawa, J. J. Mortensen, B. Hammer, J. K. Nørskov, *Surf. Sci.* 386, 67(1997)
- [7] Z.-P. Liu, P. Hu, *J. Chem. Phys.* 114, 8244 (2001)

## CO<sub>2</sub> methanation reaction on the Ni(111) surface: first-principles kinetic Monte Carlo study

P61

Pablo Lozano \*, Hèctor Prats\*, Pablo Gamallo\*, Francesc Illas\* and Ramón Sayós\*

\* *Departament de Ciència de Materials i Química Física and Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, C. Martí i Franquès 1, 08028 Barcelona, Spain.*

The proliferation of industries in the recent years have increased the amount of anthropogenic carbon dioxide emissions to the atmosphere. Since CO<sub>2</sub> is one of the main greenhouse gases that contributes to the global warming, its capture and use has become a primary task. Several reactions of industrial interest allow the transformation of CO<sub>2</sub> on important reactants such as CO, CH<sub>2</sub>O, CH<sub>3</sub>OH, CH<sub>4</sub> among others. By means of heterogeneous catalysis, CO<sub>2</sub> is hydrogenated to methane using Ni-based catalysts [1], which are known to be active for CO<sub>2</sub> methanation. In fact, they are the most widely used materials in industry due to the good balance between cost and activity. In our first study we have focused on the competition between the hydrogenation of carbon dioxide to produce methane (i.e., Sabatier reaction) against the production of carbon monoxide (i.e., reverse Water Gas Shift reaction) on the Ni (111) surface. Some experimental and theoretical studies [2,3,4] have focused on the Ni (111) surface because it is the most common and stable face for nickel catalysts and a good benchmark to study the Sabatier reaction. We have characterized all the energy barriers and adsorption energies involved in all the surface elementary processes on the nickel (111) surface, by means of Density Functional Theory (DFT) calculations using the BEEF-VdW functional, which accounts from dispersion contributions. Kinetic Monte Carlo (kMC) simulations have also been performed to account for the kinetics of this system and to give some insights about differing competing mechanisms. We have done kMC simulations with a total number of 50-60 elementary steps considering surface reactions, surface diffusions and adsorption/desorption processes. Moreover, lateral interactions between the most important intermediate species are considered to better describe the system. The simulations were carried out using several temperatures and partial pressures for CO<sub>2</sub> and H<sub>2</sub> to mimic the experimental conditions [4]. Rate constants for all processes were obtained from DFT data along with transition state theory or collision theory. From our kMC simulations, we conclude that reverse Water Gas Shift reaction is more likely to occur on nickel (111) surface than the Sabatier reaction and that not carbon deposition is observed. This suggests that CO<sub>2</sub> methanation should be occurring mainly through steps and defects of the Ni surfaces.

- [1] K. Jalama., Catal Rev, 59, 2017, page 1
- [2] Choe et al., Bull Korean Chem. Soc. 26, 2005, page 1682
- [3] Ren et al., Appl. Surf. Sci, 351, 2015, page 504
- [4] Heine et al., J. Am. Chem. Soc. 138, 2016, page 13246

---

## Unraveling Morphological and Topological Key Aspects of Pd Nanoparticles

P62

Lorena Vega\*, Francesc Viñes\* and Konstantin M. Neyman\*,†

\* *Universitat de Barcelona, 08028 Barcelona, Spain*

† *ICREA (Institució Catalana de Recerca i Estudis Avançats) 08010 Barcelona, Spain*

Metal nanoparticles (NPs) are relevant to heterogenous catalysis due to their properties, distinct from those of single-crystal surfaces and bulks. A key aspect of interest is the size-dependent

evolution of the NPs properties towards the bulk limit [1], including their geometric structures. In fact, both the shape and NP energetic stability may drastically change with NP size. Here we investigate the stability with size of different Pd NP shapes, systems of paramount importance in heterogeneous catalysis [2]. Apart from Wulff constructions, we consider other shapes so as to unfold how atomic sites with different coordination number (CN), such as corner, edge, facets, or bulk-like positions are affecting the energetic stability, allowing a breakdown of the energy by these topological contributions [3].

In particular, Pd<sub>n</sub> NPs with n = 14-1504 atoms and different shapes have been studied, including Cubes, Truncated Cubes, Octahedrons, Truncated Octahedrons, Cuboctahedrons, Icosahedrons, and Spheres, showing some preference of given shapes, although the results reveal the possible coexistence of different shapes across large regions of size. All electron Density Functional Theory (DFT) calculations have been possible by using the FHI-AIMS code [4], allowing for a massive parallelization of the optimizations using supercomputing facilities. The Perdew-Burke-Ernzerhof (PBE) functional was used for the calculations given it is a good compromise between the accuracy and the computational time. Actually, it has been proven to be one of the best choices when describing transition metals bulk and surface properties [5].

- [1] F. Viñes, F. Illas, K.M. Neyman, *J. Phys. Chem. A* 112 (2008) 8911.
- [2] S.M. Kozlov, K.M. Neyman, *J. Catal.* 337 (2016) 111.
- [3] S.M. Kozlov, G. Kovács, R. Ferrando, K.M. Neyman, *Chem. Sci.* 6 (2015) 3868.
- [4] V. Blum *et al.*, *Comput. Phys. Commun.* 180 (2009) 2175.
- [5] L. Vega, J. Ruvireta, F. Viñes, F. Illas, *J. Chem. Theory Comput.* 14 (2018) 395.

---

## Subsurface Carbon: A General Feature of Noble Metals

P63

Oriol Piqué\*, Iskra Z. Koleva<sup>†</sup>, Francesc Viñes\*, Hristiyan A. Aleksandrov<sup>†</sup>, Georgi N. Vayssilov<sup>†</sup>  
and Francesc Illas\*

\* *Departament de Ciència de Materials i Química Física & Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, c/ Martí i Franquès 1, Barcelona 08028, Spain*

<sup>†</sup> *Faculty of Chemistry and Pharmacy, University of Sofia, 1126 Sofia, Bulgaria*

Carbon C<sub>n</sub> moieties on late transition metals are historically regarded as poisoning agents for their use in heterogeneous catalysis.<sup>[1]</sup> Recent experimental studies combining *ab initio* simulations showed the promoting catalytic role of subsurface C atoms in Pd surfaces,<sup>[2]</sup> plus their existence was well established in Ni and Pt surfaces.<sup>[3]</sup> Here we show, adjoining energetic and kinetic evidences obtained by accurate density functional simulations on surface and nanoparticle models, that such subsurface C species are a general issue to be considered even in coinage noble metal systems.<sup>[4]</sup> Subsurface C is the most stable situation in densely packed (111) surfaces of Cu and Ag, with sinking barriers low enough to be overcome at catalytic working temperatures. Low-coordinated sites at nanoparticles edges and corners further stabilize them, even in gold, with negligible subsurface sinking barriers. The malleability of low-coordinated sites appears to be the key aspect in the subsurface C accommodation. The incorporation of C species decreases the electron density of the surrounding metal atoms, thus affecting their chemical and catalytic activity. These results broaden the subsurface C chemistry, so as to be considered a general aspect to be regarded in future studies on heterogeneously catalyzed processes by late transition metal systems.

- [1] S. K. Sengar, B. R. Mehta, R. Kumar, V. Singh, *Sci. Rep.*, **2013**, *3*, 2814.  
 [2] D. Teschner, J. Borsodi, A. Wootsch, Z. Révay, M. Hävecker, A. Knop-Gericke, S. D. Jackson, R. Schlögl, *Science*, **2008**, *320*, 86.  
 [3] P. Janthon, F. Viñes, J. Sirijaraensre, J. Limtrakul, F. Illas, *Catal. Sci. Technol.*, **2017**, *7*, 807.  
 [4] O. Piqué, I. Z. Koleva, F. Viñes, H. A. Aleksandrov, G. N. Vayssilov, F. Illas, *Angew. Chem.*, **2019**, *58*, 1744.

---

## Morphology Dependence of Stability and Properties of Stoichiometric TiO<sub>2</sub> Nanoparticles

P64

Ángel Morales-García\*, Antoni Macià\*, Stefan T. Bromley\*,<sup>†</sup> and Francesc Illas\*

\* *Departament de Ciència de Materials i Química Física. Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, c/ Martí i Franques 1-11, 08028 Barcelona, Spain*

<sup>†</sup> *Institució Catalana de Recerca i Estudis Avançats (ICREA), Passeig Lluís Companys 23, 08010 Barcelona, Spain*

Hydrogen constitutes an ideal green fuel but so far it is mainly obtained from fossil resources. Water splitting using TiO<sub>2</sub> as a photocatalyst constitutes an alternative although its practical use under visible sunlight is hindered from the too large “band gap” of the known forms of this oxide. Suitable modifications have been proposed including doping and/or nanostructuring. Nevertheless, finding a practical solution without a deep knowledge of how the properties of TiO<sub>2</sub> nanoparticles evolve with size, shape and morphology seems to be an insurmountable task. To make progress in this direction, a systematic study has been carried out regarding the relative stability and properties of differently shaped realistic (TiO<sub>2</sub>)<sub>n</sub> nanoparticles containing explicitly up to 1785 atoms or 595 formula units. Using all electron, relativistic, density functional theory-based calculations with accurate numerical orbital centered basis sets,[1] we investigated the relative stability of spherical and faceted nanoparticles as a function of size. A crossover between faceted and spherical morphology is found at 100 TiO<sub>2</sub> units where the faceted nanoparticles become more stable than the spherical ones. The present study provides compelling evidence that for stoichiometric nanoparticles of realistic size, a faceted morphology is preferred although spherical shaped ones tend to exhibit smaller optical gap.[2] Therefore, the successful synthesis of spherical nanoparticles, often showing better photocatalytic activity, has to be attributed to the particular route used able to stabilize these energetically metastable structures. The present study suggests that controlling kinetic of particle growth rather than thermodynamic stability is the key towards TiO<sub>2</sub> nanoparticles with better photocatalytic activity under sunlight.

- [1] Blum et al., *Comput. Phys. Commun.*, **180**, 2009, 2175  
 [2] Morales-García et al., *Nanoscale*, DOI:10.1039/C9NR00812H

---

## Entanglements and Information Theoretic Measures in Nanostructure Systems

P65

pooja<sup>\*</sup>, Rama Gupta<sup>†</sup> and Anil Kumar<sup>‡</sup><sup>\*</sup> *DAV University, Jalandhar*<sup>†</sup> *DAV University, Jalandhar*<sup>‡</sup> *JC DAV College, Dasuya*

Systems based on quantum-dot nanostructures could be used as components for quantum information processing devices. One of the possible advantages of the use of quantum dots is that the parameters of the system may be changed, allowing the properties of semiconductor nanostructures to be tailored. To use quantum dot devices for quantum computing necessitates the ability to generate and manipulate entanglement within these structures. In quantum dot systems this entanglement could be controlled through externally applied electro-magnetic fields or by varying the parameters of the nanostructure. Since entanglement is considered a key ingredient for quantum information processes, ascertaining the availability of entanglement in these nanostructures would appear to be useful when designing them. However it is often practically impossible to exactly model many-electron systems, such as complex nanostructures, and therefore precisely calculate their entanglement degree.

We investigate the use of the position space information entropy as an indicator of the entanglement for this system. Shannon information entropy is a fundamental quantity, closely related to thermodynamical entropy, which measures the spread or extent of the single particle density [1]. Information entropy plays a crucial role in a stronger formulation of the uncertainty relations. Using Supersymmetric Quantum mechanics, isospectral Hamiltonian approach is utilized to calculate the information entropy of the isospectral potential which contain a free parameter. This free parameter can be adjusted to model the complex nanostructure materials and therefore precisely calculate their entanglement degree.

[1] C.E. Shannon, W. Weaver, The mathematical theory of communication, University of Illinois Press, Urbana 1949.

[2]

---

## Thermal Transport in Si/Ge Nano-Grains using Ab-initio Simulations

P66

Alaa Akkoush<sup>\*</sup><sup>\*</sup> *American University of Beirut*<sup>†</sup> *Fritz Haber Institute*

In this work, we intend to design nano-granular meta-materials in which phonon boundary scattering mechanisms induce strong reduction in the lattice thermal conductivity. Such systems are expected to show high thermoelectric figure of merit and contribute significantly to the efforts done so far to develop alternative energy technologies.

We present a solution for spatial dependent Boltzmann equation within the single mode relaxation time approximation yielding an accurate expression for thermal conductivity of nano-sized materials or nano-grains. Upon using the conservation of heat flux theorem, we develop an expression for thermal conductivity of a monolayer of nano-grains. Then, we use the Diffuse Mismatch Model (DMM) to develop an expression for thermal conductivity of granular materials. The relaxation times are derived from Fermi's golden rule and the harmonic and anharmonic terms of the force constants involved in the model are derived from first principles techniques.

We apply our model to calculate the thermal conductivity of a granular material made up of a mixture of nano-grains of silicon and germanium. The results demonstrate that such a material is characterized by a thermal conductivity as low as the thermal conductivity of SiGe alloy, which is a well-established thermoelectric material for application in environments of very high temperatures. We demonstrate that the mixture of silicon and germanium nano-grains can be more convenient than SiGe alloy in thermoelectric applications, as they do not present the alloys structure stability problems.

- [1] C. Glassbrenner and G. A. Slack, "Thermal conductivity of silicon and germanium from 3 k to the melting point," *Physical Review*, vol. 134, no. 4A, p. A1058, 1964.
- [2] G. J. Snyder and E. S. Toberer, "Complex thermoelectric materials," in *Materials For Sustainable Energy: A Collection of Peer-Reviewed Research and Review Articles from Nature Publishing Group*, pp. 101 – 110, World Scientific, 2011.
- [3] P. Reddy, K. Castelino, and A. Majumdar, "Diffuse mismatch model of thermal boundary conductance using exact phonon dispersion," *Applied Physics Letters*, vol. 87, no. 21, p. 211908, 2005.

---

## ***In silico* characterisation of anharmonic free energies of molecular crystals**

P67

Marcin Krynski\* and Mariana Rossi\*

\* *Fritz Haber Institute of the Max Planck Society*

Organic molecular crystals are a vast group of compounds with undisputed industry importance, known for their ability to form polymorphs with properties tied strongly to their crystallographic structure. It is then of utmost importance to differentiate between those forms by establishing a relative stability ranking. A large body of theoretical research is centered on creating such a ranking [1], which is impacted by the (often neglected) thermodynamic conditions and anharmonicities of the potential energy surface.

Here we present an automated framework for the prediction of anharmonic free energies in molecular crystals. We employ dispersion-corrected density-functional theory and compare full anharmonic free-energy evaluations [2] to more computationally tractable approximate methods, gauging the effect of lattice expansion at different temperatures. To achieve an *ab initio*-quality high-throughput framework, we apply a local Gaussian process regression model to predict harmonic free energies, as well as the difference between anharmonic free energies from empirical force-fields and density-functional theory potential energy surfaces.

- [1] A. Reilly et al., *Acta Cryst. B* 72, 439 (2016);

[2] M. Rossi, P. Gasparotto, M. Ceriotti, PRL 117, 115702 (2016)

---

## Electrochemical doping of HfNCl: spin-orbit coupling, spin texture, and Ising superconductivity

P68

Thomas Brumme\*, Matteo Calandra<sup>†</sup> and Francesco Mauri<sup>‡</sup>

\* *Wilhelm-Ostwald-Institute of Physical and Theoretical Chemistry, Leipzig University, Leipzig, Germany*

<sup>†</sup> *CNRS, UMR 7590, Sorbonne Universités, UPMC Univ Paris 06, IMPMC, Paris, France*

<sup>‡</sup> *Dipartimento di Fisica, Università di Roma La Sapienza, Roma, Italy*

The transition-metal dichalcogenides (TMDs) have received a lot of attention as possible candidates to build valleytronic devices in which the valley degree of freedom is used to store and process information. In recent years it became furthermore possible to dope these layered materials in the order of  $10^{14}$  charge carriers  $\text{cm}^{-2}$  using ionic-liquid based field-effect transistors. This allows for the exploration of the semiconducting, metallic, superconducting, and charge-density-wave regimes in reduced dimensionality. Additionally, as the spin is polarized perpendicularly to the layer for charge carriers in the spin-orbit split band extrema, TMDs show so-called Ising superconductivity: electrons with opposite out-of-plane spins in opposite K and K' valleys form singlet Cooper pairs, thus increasing the upper critical field that is needed to destroy the superconducting state. The related transition-metal chloronitride HfNCl is usually not considered in this context, as the bands are not spin-orbit split due to the presence of inversion symmetry. Yet, in a field-effect setup the asymmetric external electric field leads to a breaking of the inversion symmetry. We calculated within density-functional theory the band structure and spin-orbit splitting for field-effect doped HfNCl. We show how the external electric field leads to changes in the spin texture in the conduction band minimum and estimate the in-plane, upper critical field  $H_{c2}^{\parallel}$ .

- [1] J. M. Lu, O. Zheliuk, I. Leermakers, N. F. Q. Yuan, U. Zeitler, K. T. Law & J. T. Ye, *Science* 350, 1353 (2015)
- [2] X. Xi, Z. Wang, W. Zhao, J.-H. Park, K. T. Law, H. Berger, L. Forró, J. Shan & K. F. Mak, *Nat. Phys.* 12, 139 (2016)
- [3] S. C. de la Barrera, M. R. Sinko, D. P. Gopalan, N. Sivadas, K. L. Seyler, K. Watanabe, T. Taniguchi, A. W. Tsen, X. Xu, D. Xiao & B. M. Hunt, *Nat. Commun.* 9, 1427 (2018)
- [4] T. Brumme, M. Calandra & F. Mauri, *Phys. Rev. B* 89, 245406 (2014)
- [5] T. Brumme, M. Calandra & F. Mauri, *Phys. Rev. B* 91, 155436 (2015)
- [6] T. Brumme, M. Calandra & F. Mauri, in preparation

---

## Second-order Møller-Plesset perturbation theory and beyond for the band gap and single-particle excitations of solids

P69

Maria Dragoumi\*, Sergey V. Levchenko<sup>†,‡</sup>, Igor Ying Zhang<sup>4</sup> and Matthias Scheffler\*

\* *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin*

† *Skolkovo Innovation Center, Moscow*

‡ *NUST MISIS, Moscow*

<sup>4</sup> *Fudan University, Shanghai*

Calculations of the fundamental band-gap and the low-energy excitations of solids are still a challenge for electronic-structure theory. The computationally efficient Kohn-Sham (KS) density functional theory (DFT) with the widely used local or semi-local approximations provides a KS band gap which is much smaller than the fundamental gap. Many-body perturbation theory, on the other hand, addresses the fundamental gap directly. We present here an efficient scalable implementation of Møller-Plesset second order perturbation theory (MP2) for quasi-particle energies [1,2]. By solving the Dyson equation of the single-particle Green's function, considering self-energy up to second order, we go beyond MP2. The new approach shows a competitive or even superior performance in comparison to the current state-of-the-art methods such as hybrid functionals and approximation, where second order exchange is missing. We present numerical results for the band-gap of a wide range of semiconductors and insulators.

1 J. Sun and R. J. Bartlett, *J. Chem. Phys.* 104, 8553 (1996).

2 A. Grüneis, et.al, *J. Chem. Phys.* 133, 074107 (2010).

---

## Representations of molecules and materials for interpolation of ab initio calculations

P70

Marcel Langer\*, Alex Goessmann<sup>†</sup> and Matthias Rupp<sup>\*,‡</sup>

\* *Fritz Haber Institute of the Max Planck Society, Berlin, Germany*

† *Technische Universität Berlin, Germany*

‡ *Citrine Informatics, Redwood City, California, USA*

High-throughput applications, such as the search for novel materials, drug screening, or the exploration of phase diagrams require first principles simulations of molecules and materials, but are limited by their high computational cost. Interpolating between reference calculations, machine learning can act as a fast and accurate surrogate, greatly increasing the number of accessible systems. [1] This requires a *representation* of molecules and materials suitable for interpolation.

We benchmark the predictive accuracy of selected state-of-the-art representations by carefully controlling for all other factors influencing performance, including data distribution, regression method and hyper-parameter optimisation. For the latter, we employ a consistent and automatic procedure to optimise both numerical and categorical free parameters using sequential model-based



optimisation with tree-structured Parzen estimators. [2] We also investigate how the representations can be understood in a unified framework [3] based on  $k$ -body functions, group averaging and tensor products, and discuss implications.

- 1 a) M. Rupp et al., Phys Rev Lett 108 (2012) 058301. b) M. Rupp, Int J Quant Chem 115 (2015) 1058.
- 2 a) J.S. Bergstra et al., NIPS 24 (2011) 2546. b) J.S. Bergstra et al., ICML 30 (2013) I-115.
- 3 M.J. Willatt, F. Musil, M. Ceriotti, arXiv (2018) 1807.00408.

## Interplay of quantum nuclear fluctuations and the electronic structure of the cyclohexane/Rh(111) interface

P71

Karen Fidanyan\* and Mariana Rossi\*

\* *Fritz Haber Institute of the Max Planck Society*

Cyclohexane ( $C_6H_{12}$ ) adsorbed on metal surfaces can participate in catalytic dehydrogenation reactions, which show good potential for hydrogen storage. It has been observed experimentally that  $C_6H_{12}$  adsorbed on the Rh(111) surface shows an isotope effect on the work function change and the adsorption energy upon deuteration [1]. The physical origin of this puzzling isotope effect on the electronic structure has not been fully resolved. We employ density-functional theory (PBE functional with van der Waals corrections) and *ab initio* path-integral molecular dynamics at 150 K to characterize the underlying physics of this phenomenon. We perform these simulations almost at classical-nuclei cost by making use of the spatially-localized ring-polymer contraction scheme proposed in Ref. [2]. The harmonic approximation to zero-point-energy in the adsorption energy is not able to capture the isotope effects observed experimentally. We thus include anharmonic corrections through the dynamics and identify the temperature-dependent electronic level broadening and renormalization due to the interaction with phonons in this system.

[1] Koitaya T. and Yoshinobu J., Chem. Rec. 14 848-856 (2014).

[2] Litman Y., Donadio D., Ceriotti M. and Rossi M., J. Chem. Phys. 148 102320 (2018).

## Interplay of quantum nuclear fluctuations and the electronic structure of the cyclohexane/Rh(111) interface

P72

Karen Fidanyan\* and Mariana Rossi\*

\* *Fritz Haber Institute of the Max Planck Society*

Cyclohexane ( $C_6H_{12}$ ) adsorbed on metal surfaces can participate in catalytic dehydrogenation reactions, which show good potential for hydrogen storage. It has been observed experimentally that  $C_6H_{12}$  adsorbed on the Rh(111) surface shows an isotope effect on the work function change and

the adsorption energy upon deuteration [1]. The physical origin of this puzzling isotope effect on the electronic structure has not been fully resolved. We employ density-functional theory (PBE functional with van der Waals corrections) and *ab initio* path-integral molecular dynamics at 150 K to characterize the underlying physics of this phenomenon. We perform these simulations almost at classical-nuclei cost by making use of the spatially-localized ring-polymer contraction scheme proposed in Ref. [2]. The harmonic approximation to zero-point-energy in the adsorption energy is not able to capture the isotope effects observed experimentally. We thus include anharmonic corrections through the dynamics and identify the temperature-dependent electronic level broadening and renormalization due to the interaction with phonons in this system.

[1] Koitaya T. and Yoshinobu J., *Chem. Rec.* 14 848-856 (2014).

[2] Litman Y., Donadio D., Ceriotti M. and Rossi M., *J. Chem. Phys.* 148 102320 (2018).

---

## Fully-Anharmonic, First-Principles Theory of Electronic Transport

P73

Zhenkun Yuan\*, Marios Zacharias\*, Matthias Scheffler\* and Christian Carbogno\*

\* *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin*

Under typical operation conditions, thermoelectric charge and heat transport are limited by scattering events resulting from electron-phonon coupling (EPC). Although much progress has been made in assessing the respective electronic transport coefficients in the harmonic approximation [1], recent evidence suggests that anharmonic contributions both in the nuclear motion *and* the EPCs can play a decisive whereas typically ignored role [2]. We here present a first-principles formalism that fully accounts for these anharmonic effects in electronic transport: Anharmonicity in the nuclear motion is accounted for via *ab initio* molecular dynamics, while anharmonicity in the EPCs is included by evaluating the electronic self-energy along these trajectories in a real-time density-matrix formalism. This gives access to the electronic charge and heat fluxes, enabling us to obtain the thermoelectric transport coefficients via the fluctuation-dissipation theorem. Using both harmonic elemental semiconductors and anharmonic perovskites as example, we discuss the advantages and challenges of the proposed approach.

[1] S. Ponc e, E. R. Margine, and F. Giustino, *Phys. Rev. B* **97**, 121201 (2018)

[2] J.-J. Zhou, O. Hellman, and M. Bernardi, *arXiv:1806.05775* (2018)

---

## Blueprint strategy for cation-peptide force-field parameterization

P74

Xiaojuan Hu\*, Markus Schneider\* and Carsten Baldauf\*

\* *Fritz-Haber-Institut der Max-Planck-Gesellschaft*

Nearly half of all proteins contain metal ions, which perform a wide variety of specific functions associated with life's processes. Metallothioneins (MTs) are a family of low-molecular weight, cysteine-rich, and metal-rich proteins present in all living organisms. They are of great interest to study because of their importance in physiology and roles in various diseases. However a central aspect of their function, e.g. metal-ion release, is not yet fully understood. It is the aim of this project to pave the way towards a detailed understanding of metalloprotein structure, function, and dynamics. Force fields are typically used in molecular-dynamics simulations. We tested the accuracy of force fields by comparing to potential energies from CCSD(T) calculations (<http://arxiv.org/abs/1810.10596>). The result showed that the errors of force fields describing cation-peptide interactions appear extremely large. The errors may stem from two reasons: (1) The force field parameters were derived for condensed phase systems, while we are considering gas phase; (2) standard force fields do not take charge transfer and polarization effects into account. To improve the accuracy of force fields, we develop a regression scheme for the system-specific parametrization of metal-cation potentials based on energies from electronic-structure theory calculations. We illustrate the approach with an exploratory study on the alanine dipeptide alone and with a sodium cation as well as on deprotonated cysteine (Ace-Cys<sup>-</sup>-NME) alone and with a Zn-cation. Our re-parametrizations eventually yield drastic improvements, yet particularly when including cations, we cannot reach the magical border of 1 kcal/mol chemical accuracy, arguably due to the fixed partial-charge model and angle distortions. To make the charge fluctuant and compensate for the angle distortion, charge transfer and polarization will be included for the non-bonded interactions in the Zn-ligand sphere based on the updated partial charges and the extension of classical force fields with polarization energy.

[1] <http://arxiv.org/abs/1810.10596>

---

## Accelerating the High-Throughput Search for Strongly Anharmonic Thermal Insulators

P75

Thomas Purcell\*, Florian Knoop\*, Matthias Scheffler\* and Christian Carbogno\*

\* *Theory Department, Fritz Haber Institute*

Finding materials with lower thermal conductivities  $\kappa$  is necessary for many applications, such as thermoelectricity. Since  $\kappa$  is limited by phonon scattering, this implies identifying strongly anharmonic materials and accurately studying them by accounting for anharmonic effects via *ab initio* molecular dynamics [1]. For a rapid, high-throughput screening of potential materials, this approach is however computationally too costly. It is thus desirable to accelerate the high-throughput screening for poor thermal conductors by developing an easily calculable measure of a material's anharmonicity.

In this work, we achieve this goal with a new, hierarchical, high-throughput framework. This framework combines the Atomic Simulation Environment (ASE) [2] with FireWorks [3] and FHI-Aims [4] to calculate the harmonic force constants of a broad set of materials ranging from simple group-V semiconductors to complex perovskites in an automated fashion. Anharmonicity is then quantified by inspecting the differences between harmonic and actual forces observed for geometries in thermal equilibrium. This extensive data set, covering a thousand materials and a hundred thousand first-principles calculation is then analysed using SISSO (sure independence screening

and sparifying operator) [5] to create a new descriptor for anharmonicity. This descriptor is further validated by extended ab initio MD calculations.

- [1] 1. C. Carbogno, R. Ramprasad, and M. Scheffler. *Phys. Rev. Lett.* **118**. 175901 (2017).
- [2] 2. A. S. Larsen, et al. *J. Phys. Condens. Matter.* **29**. 273002 (2017)
- [3] 3. A. Jain, et al. *Concurrency Computat. Pract. Exper.* **27**. 5037 (2015)
- [4] 4. V. Blum, et al. *Comp. Phys. Comm.* **180**. 2175 (2009).
- [5] 5. R. Ouyang, S. Curtarolo, E. Ahmetcik, M. Scheffler, and L.M. Ghiringhelli. *Phys. Rev. Mat.* **2**. 083802 (2018)

# 4 List of Participants

## Speakers

Volker	Blum	volker.blum@duke.edu
Christian	Carbogno	carbogno@fhi-berlin.mpg.de
David	Casanova	
Stefano	Curtarolo	stefano@duke.edu
Claudia	Draxl	claudia.draxl@physik.hu-berlin.de
Luca	Ghiringhelli	ghiringhelli@fhi-berlin.mpg.de
Morten	Gjerdning	mogje@fysik.dtu.dk
Andreas	Grüneis	andreas.grueneis@tuwien.ac.at
Björk	Hammer	hammer@phys.au.dk
Geoffroy	Hautier	
Nicholas	Hine	N.D.M.Hine@warwick.ac.uk
Paul	Kent	kentpr@ornl.gov
Florian	Knoop	knoop@fhi-berlin.mpg.de
Peter	Kratzer	peter.kratzer@uni-due.de
Ask Hjorth	Larsen	asklarsen@gmail.com
Sergey V.	Levchenko	levchenko@fhi-berlin.mpg.de
Miguel Alexandre	Marques	
Nicola	Marzari	nicola.marzari@epfl.ch
Nikolaj	Moll	nim@zurich.ibm.com
Danny	Perez	danny_perez@lanl.gov
Xinguo	Ren	renxg@ustc.edu.cn
Karsten	Reuter	karsten.reuter@ch.tum.de
Patrick	Rinke	patrick.rinke@aalto.fi
Erich	Runge	Erich.Runge@TU-Ilmenau.de
Stefano	Sanvito	sanvitos@tcd.ie
Matthias	Scheffler	scheffler@fhi-berlin.mpg.de
Susan	Sinnott	sinnott@matse.psu.edu
Alexandre	Tkatchenko	alexandre.tkatchenko@uni.lu
Mateo	Valero	mateo.valero@bsc.es
Scott M.	Woodley	Scott.Woodley@ucl.ac.uk
Weitao	Yang	weitao.yang@duke.edu

## Tutors

Alaa	Akkoush	akkoush@fhi-berlin.mpg.de
Nikita	Rybin	n.seryh@gmail.com
Daniel	Speckhard	speckhard@fhi-berlin.mpg.de
Marcin	Krynski	krynski@fhi-berlin.mpg.de
Thomas	Brumme	thomas.brumme@uni-leipzig.de

## 4 List of Participants

Maria	Dragoumi	dragoumi@fhi-berlin.mpg.de
Dmitrii	Maksimov	maksimov@fhi-berlin.mpg.de
Marcel	Langer	langer@fhi-berlin.mpg.de
Karen	Fidanyan	fidanyan@fhi-berlin.mpg.de
Zhenkun	Yuan	yuan@fhi-berlin.mpg.de
Sara	Panahian Jand	panahianjand@fhi-berlin.mpg.de
Xiaojuan	Hu	xhu@fhi-berlin.mpg.de
Thomas	Purcell	purcell@fhi-berlin.mpg.de
Dorothea	Golze	dorothea.golze@aalto.fi

### Organizers

Francesc	Illas Riera	francesc.illas@ub.edu
Eliseo	Ruiz Sabin	eliseo.ruiz@qi.ub.es
Silvia	Chellini	schellini@ub.edu
Sebastian	Kokott	kokott@fhi-berlin.mpg.de
Carsten	Baldauf	baldauf@fhi-berlin.mpg.de
Volker	Blum	volker.blum@duke.edu
Matthias	Scheffler	scheffler@fi-berlin.mpg.de

### Students

Aleksandra	Oranskaia	aleksandra.oranskaia@kaust.edu.sa
Kathleen	Mullin	kathleenmullin2023@u.northwestern.edu
shabnam	naseri	shabnam.naseri@ltu.se
Karla	Andriani	karlandrianiqmc@gmail.com
Alena	Vishina	alena.vishina@physics.uu.se
Jéssica	Santos Rego	jrego@ifi.unicamp.br
Mahmoud	Mansi	mansim@cardiff.ac.uk
Evgeny	Kadilenko	emkad@yandex.ru
Kyle	Miller	kmiller@u.northwestern.edu
Gustav	Johansson	gustav.johansson@ltu.se
Daniele	Perilli	d.perilli@campus.unimib.it
Sri Harsha	Pulumati	shp16@hi.is
Aurelio	Gallardo	aureliogaca@fzu.cz
Shayan	Edalatmanesh	shyn.ein@gmail.com
Alessandro	Stroppa	alessandro.stroppa@spin.cnr.it
Mehdi	Nourazar	mehdin@kth.se
Oscar	Toledano	otoledano@ccia.uned.es
Martin	Liebetau	liebetau.martin@gmail.com
Soumyadipta	Sengupta	s.sengupta@tue.nl
Roman	Kempt	r.kempt@hzdr.de
Tommaso	Civitarese	tommaso.civitarese@uniroma1.it
Samuel	Young	samueldy@umich.edu
Masoud	Mansouri	ma.mansouri@dipc.org
Panagiotis Pavlos	Stavroulakis	ppstavroulakis1@sheffield.ac.uk
Can	Kocer	cpk27@cam.ac.uk
Magnar	Björgve	magnar.bjorgve@uit.no

## 4 List of Participants

Katawoura	Beltako	katawoura.beltako@oist.jp
Shuai	Dong	sdong@seu.edu.cn
León-Alexander	Martin	leon.martin@uni-konstanz.de
Yuta	Ito	yuta.ito@oist.jp
Andrea	Grisafi	andrea.grisafi@epfl.ch
Carlos Manuel	de Armas Morejon	carlosdearmasm@gmail.com
Guangzong	Xing	guangzong.xing@oist.jp
Asbjoern	Burow	asbjoern.burow@avmatsim.eu
Simon	Anniés	simon-annies@web.de
John	Lasseter	lasseterjc@ornl.gov
Byung-Hyun	Kim	bhkim@kier.re.kr
Chan-Woo	Lee	cwandtj@kier.re.kr
Bandar	AlOtaibi	bmalotaibi@kacst.edu.sa
Leonel	Llanos	leonel.llanos@usach.cl
Eliel	Silva Neto	elielgsn@gmail.com
Jorge	Laranjeira	jorgelaranjeira@ua.pt
Quang Thang	Trinh	qttrinh@ntu.edu.sg
Matthias	Golomb	mjg3518@ic.ac.uk
Tyler	Whitaker	tylervw@byu.edu
Brayden	Bekker	brayden.bekker@byu.edu
Hadi	Arefi	h.arefi@fz-juelich.de
Han Seul	Kim	hanseulkim0@gmail.com
Maxime	MAURICE	maxime.maurice@promes.cnrs.fr
Pouya	Partovi-Azar	pouya.partovi-azar@chemie.uni-halle.de
Sandeep	Kumar	sandeep.kumar@uni.lu
Tatiana	Kostiuchenko	Tatiana.Kostiuchenko@skoltech.ru
Daniel	Schwalbe-Koda	dskoda@mit.edu
Xingyu	Liu	xingyull@andrew.cmu.edu
Billal	Sohail	billal.sohail@warwick.ac.uk
Hanna	Tuerk	hanna.tuerk@tum.de
Frederic	Felsen	frederic.felsen@tum.de
Julius	Hornung	julius.hornung@tum.de
Vivianne Karina	Ocampo Restrepo	vivianne.o.restrepo@usp.br
Priscilla	Felício Sousa	priscillafelicio@usp.br
Jorge Andres	Navarro Giraldo	jorge.navarro@ceitec.vutbr.cz
Maximilian	Schörner	maximilian.schoerner@uni-rostock.de
Dmitry	Bocharov	bocharov@latnet.lv
Patricia	Pérez Bailac	patricia.perez@csic.es
Marcos	Rivera-Almazo	marcos.almazo19@gmail.com
Noemi	Bosio	bosio@chalmers.se
Antonio	Moreno Vicente	antonio.morenov@urv.cat
Pablo	Lozano	pablo.lozano222@gmail.com
Lorena	Vega	lvega@ub.edu
Oriol	Piqué	opique@ub.edu
FEI	WANG	fei.wang@urv.cat
Ángel	Morales	angel.morales@ub.edu

#### *4 List of Participants*

POOJA

BAKSHI SINGH

poojaphy19@gmail.com