Posters abstracts

Poster 1

Arsalan Akhtar, José Miguel Alonso Pruneda, Pablo Ordejón Rontomé

Ab initio study of oxygen vacancies in yttria stabilized zirconia (YSZ) Slab

Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193 Barcelona, Spain

The monitoring of gases with solid state sensors has become a well established practice in industry.
There are many categories of gas sensors, among them oxygen gas sensors are one of the basic gas sensors with purpose of measuring oxygen concentration in automobile exhaust to control the pollution.
In this project the main goal is to develop atomistic models of yttria stabilized zirconia (YSZ) which is promising material for electrolyte in gas sensors owing to its high ionic conductivity.
To do so we build the slab and investigate the different configurations of yttria and vacancies with appropriate surfaces.
At first step we are going to relax the structures to find out each defects formation energy using SIESTA package within framework of density functional theory (DFT) afterward we try to find out migration energies of vacancies in different configurations.
This step will be done by nudge elastic band (NEB) and Double nudged elastic (DNEB) methods in SIESTA. Next we introduce the electrodes to capture more realistic picture for evaluating the migration energies.

Poster 2

C. S. Cooper [a,b], D. Thompsett [a], A. E. Pascui [a], A. P. E. York [a], C. R. A. Catlow [a]

Combined theoretical and experimental approach to understanding Three-Way Catalysis on perovskite surfaces

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There is a long standing interest in perovskite oxides as potential alternatives to noble metals in certain catalytic applications. Here we present results of combined theoretical and experimental work on these materials. We discuss the mechanisms and activity for CO oxidation and NO reduction over base metal perovskite oxides and systematic theoretical screening of A- and B-site substitutions. The results show food agreement between theory and relevant experimental observations. We conclude that the good oxidation activity observed can largely be attributed to reactive oxygen species formed at the surface. NO reduction occurs by activation at surface oxygen vacancy sites, this activity is moderate under ideal conditions but severely limited under realistic conditions by competition with oxygen for surface vacancy sites. Computational screening indicates base metal doping can have only a limited effect on NO reduction performance. Theory and experiment show that supported PGMs, even at low loading, dramatically enhance activity.

Poster 3

N. M. Fortunato, I. Opahle, O. Guttfleisch and H. Zhang

High-throughput study of Heusler Alloys for Energy Applications

Institute of Materials, TU Darmstadt, Darmstadt, Germany

Heusler alloys are multi-functional materials with a wide range of potential applications, among them permanent magnets and magnetic refrigeration, which are relevant for energy efficient industrial and commercial processes. A great deal of experimental effort has been put into exploiting the Heusler family's large number of possible compositions and substitutional disorder. To accelerate this search we perform a high-throughput Density Functional Theory screening of material properties of stoichiometric all-*d*-metal based Heuslers and MM'X (M=metal, X= main group) hexagonal/orthorhombic compounds *[J. Phys. D: Appl. Phys 51, 464005 (2017)]*, looking at the stability of the martensite and austenite phases.

Further, permanent magnet relevant properties like tetragonality, magnetic anisotropy energy, saturation magnetization and Curie temperature are calculated. We found 192 stable all-*d*-metal Heusler alloys where the martensite is the lower energy phase, of which 44 are also stable in the austenite. To elucidate the feasibility of these compounds as magnetocaloric materials we look at the Bain path, magneto-volume coupling *[Chem. Mater. 29, 1613 (2017)]*, mechanical stability and interplay of magnetic and structural transition temperatures estimates.

Poster 4

F. Ellinger [a], C. Franchini [b]

High-throughput *GW* Calculations

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b Department Computational Materials Physics

In our work we implement a semi-automatized schema for calculating well converged band gaps on *GW* level of a large material dataset. The conventional approach to performing this kind of calculations requires a huge amount of computational resources and user interaction, inhibiting the efficient analysis of larger datasets. Employing a basis set extrapolation method, proposed by Klimeš et al. *[Phys. Rev. B 90, 075125]*, makes it possible to significantly reduce the time and workload necessary for achieving a converged band gap, even for large and complicated systems like perovskites. *[Phys. Rev. Materials 2, 024601]* Applying this approach, it is possible to derive a reliable method for conveniently performing a whole series of *GW* calculations, while requiring only a minimum of input files and user interference. This could speed up the production rate of *GW* level data to a scale, where large data repositories for these calculations can be created and quickly expanded. Using this procedure, we have constructed a preliminary database which, among other properties, collects *GW* band gaps. Since the data set is reasonably extensive, data driven methods could be applied to find new ways of calculating accurate band gaps. The vision would be to find a way of estimating the quasi-particle shift and thus the gap at *GW* level only with knowledge of DFT data, similar as approaches that can already be found in the literature. *[npj Computational Materials (2017) 3:54]*

Poster 5

M. Foscato, V. R. Jensen

Automated design of Fe(II) spin crossover compounds: a successful story

University of Bergen

Poster 6

D. Grassano [a], F. Bechstedt [b], O. Pulci [a]

Influence of anisotropy, tilt and pairing of Weyl nodes: the Weyl semimetals TaAs, TaP, NbAs, and NbP

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By means of *ab initio* band structure methods and model Hamiltonians we investigate the electronic, spin and topological properties of four monopnictides crystallizing in BCT structure.
We show that the Weyl bands around a WP W1 or W2 possess a strong anisotropy and tilt of the accompanying Dirac cones.
These effects are larger for W2 nodes than for W1 ones.
The node tilts and positions in energy space significantly influence the DOS of single-particle Weyl excitations.
The node anisotropies destroy the conventional picture of (anti)parallel spin and wave vector of a Weyl fermion.
This also holds for the Berry curvature around a node, while the monopole charges are independent as integrated quantities.
The pairing of the nodes strongly modify the spin texture and the Berry curvature for wave vectors in between the two nodes.
Spin components may change their orientation.
Integrals over planes perpendicular to the connection line yield finite Zak phases and winding numbers for planes between the two nodes, thereby indicating the topological character.

Poster 7

I. Heinz, P. Risius, A. Fabian, C. Heiliger

Convergence tests for KKR calculations using AiiDA

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The Korringa-Kohn-Rostoker Green's function method is a powerful tool for self-consistent electronic structure calculations and for obtaining densities of states, band structures, and transmission functions. To speed up self-consistent calculations, we consider a rectangular contour in the complex plane for the integration procedure. We analyze the dependence of numerical accuracy and calculation time on several parameters such as k-mesh and energy grid. For these tests, we utilize the first version of our plugin for AiiDA *[Comp. Mat. Sci 111, 218 (2016)]*, on which we are currently working.

Starting from the Jülich KKR-plugin *[https://aiida-kkr.readthedocs.io]*, we implemented our conceptualization and formatting of inputs and outputs as present in the Giessen KKR code. For now, all basic functionalities including density of states, band structure, and transport calculations are provided. To automate the calculations, we will focus on implementing workflows for all relevant use cases. We also are planning to add a new plugin for helper scripts, *e.g.* to adjust output potentials for transport geometries. We also provide an outlook on future directions.

Poster 8

M. Kar, D. Kramer

First Principles calculations of potential additives in Li-ion batteries to prevent thermal runaway

University of Southampton, Department of Mechanical Engineering

The ongoing challenge to integrate and balance renewable energy sources have created the need for innovation in energy storage. Lithium ion battery (LIB) received much attention in recent years as a high density energy store. This is mainly because of the lightness and relatively high density of the used intercalation compounds paired with large voltage differences. That makes them ideal for portable devices, such as laptops.
However, Li ion technology faces significant safety challenges for larger scale applications, such as in electric vehicles, etc., due to the increasing energy content and associated increased risk associated with failure modes in these batteries. Failure modes due to thermal, mechanical, and electrical abuse may lead to thermal runaway, with potentially lethal consequences.
In this work, we perform first principles calculations on potential additives for Li-ion batteries, that show a positive temperature coefficient of resistivity (PTCR) effect. It is expected that these additives can be used to prevent the excessive temperature rise due to abusive electrochemical charge/discharge and act as a cut-off mechanism physically preventing thermal runaway phenomena, thus improving safety of these devices.

References:

P. Ribiere, S. Grugeon, M. Morcrette, S. Boyanov, S. Laurelle and G. Marlair, Energy Environ. Sci., 5, 2012

Poster 9

Hyun-Jung Kim, Young-Woo Son

TBFIT: An open-source software package for Slater-Koster tight-binding parameter fitting

Korea Institute for Advanced Study

John von Neumann famously said “With four parameters I can fit an elephant, and with five I can make him wiggle his trunk”, meaning that with enough/proper parameters you can fit any data set. However, in general, it is remains a dark area of the Architect to find enough and proper parameter sets, at least I would say, in parameterizing tight-binding models.
In this poster, I introduce a recently developed open-source toolkit [https://github.com/Infant83/TBFIT] for fitting Slater-Koster tight-binding parameters *[Phys. Rev. 94, 1498 (1954)]* and its capability for describing essential features of low energy electronic properties of the materials with well known examples, graphene and bulk bismuth.
We show that in the help of genetic algorithm and non-linear least square fitting algorithm based on Levenberg-Marquadt method, one can easily obtain hopping parameters. We also show the topological invariant can be evaluated through Wannier charge center evaluation. For Bi bulk system, we report new tight binding parameter set, with up to six nearest neighbor hopping parameters.

Poster 10

L. Koschmieder [1], **M. Lin** [2], G. J. Schmitz [1]

Aachen Virtual Platform for Materials Processing

1 Access e.V.
2 IEHK RWTH Aachen University

Poster 11

R. Kováčik [a], Ph. Mavropoulos [b], S. Blügel [a]

Critical temperature and effective magnetic moment of Heusler alloys from first principles

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We present calculations of the critical temperature (Curie or N\'eel) and the effective magnetic moment of a large number ($\sim$200) of experimentally known stoichiometric magnetic Heusler alloys. The method of calculation comprises three steps: (i) calculation of the ground-state electronic structure within density functional theory (local spin density approximation and generalized gradient approximation) employing the Korringa-Kohn-Rostoker Green function method [Rep. Prog. Phys. 74, 096501 (2011)], (ii) extraction of exchange parameters to fit the Heisenberg model [J. Magn. Magn. Mater. 67, 65 (1987)], and (iii) Monte Carlo simulation based on the Heisenberg model. We analyze the critical temperature dependence on various parameters defining the alloys. The effective magnetic moment reflecting the degree of short range order above the critical temperature is obtained by fitting the magnetic susceptibility to the Curie-Weiss law and compared to available experimental data. Support from JARA-HPC (jara0182) is gratefully acknowledged.

Poster 12

Ruchika Mahajan, Arti Kashyap

Visualization of Quantum ESPRESSO jobs

Indian Institute of Technology Mandi, Mandi, India

Organizing Quantum ESPRESSO jobs endeavor requires in depth knowledge base of structural atom arrangement. α-MnO2 has a primitive tetragonal crystal structure with lattice parameters a = b = 9.78760 Å, c = 2.86500Å, where Mn atoms are octahedrally coordinated to six oxygen atoms.

We have formulated all calculations in the framework of DFT and its extensions, as implemented in Quantum ESPRESSO (QE) tool.

We used PAW pseudopotential to perform these calculations. Electronic and magnetic properties of α-MnO2 were evaluated by optimizing the crystal structure. Pure α-MnO2 is found to be a semiconductor with an indirect band gap of 1.1 eV. A thin film of pure α-MnO2 with different thickness was constructed following a bulk calculation.

Further, we have scheduled plan to dissociate the water molecule on different sites of the surface of α-MnO2 and then perform oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) of α-MnO2. Input variants of Quantum ESPRESSO files will be designed as an entry point for this phase. As a part of high throughput job It will follow bulk electronic calculation jobs to derive thin film. Automated Interactive Infrastructure and Database for Computational Science (AiiDA) will be implemented to organize Quantum ESPRESSO jobs, results and visualization.

Poster 13

D. Marchand, W.A., Curtin

Construction of accurate neural network potentials for atomic scale modeling of precipitate phenomena in aluminium alloys

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The Al2xxx and Al6xxx aluminum alloys are some of the most commonly used materials in existence. Both derive their strength from age hardening due to the formation of internal precipitates. These precipitates range from the θ phases in the AlCu alloys, the S phases in the AlCuMg alloys, to the Q phases found in the AlCuMgSi alloys.
While substantial experimental and theoretical work has been performed on these alloys and their mechanical properties, much remains unknown. The structures and even compositions for the S and Q phases, as well as in the precursors, are still unclear.
We discuss detailed plans to systematically construct Neural Network (NN) potentials using an appropriate set of Density Functional Theory (DFT) calculations as a training set. We then describe the use these NN potentials, along with kinetic Monte Carlo (KMC) methods, to elucidate the composition, structure and mechanical response of these precipitates. Additionally, we describe initial progress in the form of testing DFT settings, ruling out physical sources of error and the development of a high-throughput framework to manage calculations with AiiDA.

Poster 14

L-S. Medondjio, Z. Zanolli, P. Ordejón

First-Principles Approach to Model Quantum Electrochemistry in Liquid Environment

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Understanding the local structure of water at the interfaces of metallic electrodes is an essential requisite for predicting the correspondence between the macroscopic voltage and microscopic interfacial charge distribution in aqueous-based electrochemistry*[1]*. Indeed, accurate calculation of the electrostatic potential at electrically-biased metal-electrolyte interfaces is a challenge for ab initio simulations with periodic boundary conditions *[2, 3]*.
To correctly compute the effect of an external bias potential applied to truly semi infinite surfaces, we combine ab initio molecular dynamics and non Equilibrium Green's Function (NEGF) methods. The system under consideration being water molecule in contact with Au(111) surface. This framework allows
for out-of equilibrium calculation of forces and dynamics, and directly correlate to the chemical potential of the electrodes which is introduced experimentally.

References:
1 Chem. Sci. 9, 62-69 (2018).
2 Electrochim. Acta,84,3 (2012).
3 J.Cheng and M.Spirk, Phys. Chem. Chem. Phys. 14,11245 (2012)

Poster 15

G. Menichetti [a], M. Calandra [b], M. Polini [a]

Magnetic properties of few-layer $Cr_2Ge_2Te_6$: A comparative ab initio study

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b Sorbonne université, CNRS, Institut des Nanosciences de Paris, UMR7588, F-75252, Paris, France

Atomically-thin magnetic crystals have been recently isolated experimentally, greatly expanding the family of two-dimensional (2D) materials.
In this Poster we focus our attention on $Cr_2Ge_2Te_6$, presenting an extensive comparative analysis of its magnetic properties, based on *ab initio* density-functional theory (DFT).
We first show that the often-used DFT+U fails in predicting the ground-state properties of this material in both its monolayer and bilayer forms, and even more spectacularly in its bulk form. On the contrary, the use of hybrid functionals, which naturally take into account correlations between all orbitals (and not only between the *d* orbitals of Cr), yields very good account of the available experimental data.
We then calculate all the relevant exchange couplings for mono- and bi-layer $Cr_2Ge_2Te_6$ and its bulk form, comparing results obtained via different methods and/or super-cell size. In the case of bilayer $Cr_2Ge_2Te_6$, we show that two distinct second-neighbor exchange couplings emerge.
We have tried to give a detailed account of all available results in the literature (including also those for the magneto-crystalline anisotropy), comparing them with our findings, and commenting on the discrepancies.

References:
[1] Science 363, (2019)706
[2] Nature, 563 (2018) 47
[3] Nature,546 (2017) 265
[4] Nature,546(2017) 270

Poster 16

Takayuki Nishiyama

Grain Boundary Simulation with Machine Learning Interatomic Potential

Department of Materials Science and Engineering, Graduate School of Engineering. Kyoto University.

Poster 17

Daniele Ongari [1], Aliaksandr V. Yakutovich [1 2], Leopold Talirz [1 2], Berend Smit [1]

Using AiiDA for gas adsorption in nanoporous materials: open-source, reproducibility and automation

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The challenge of performing gas adsorption and separation using nanoporous materials can be seen as a purely combinatorial problem. On the one hand we have tens of industrially important applications, ranging from carbon capture to noble gasses separation. On the other hand we have thousands of new nanoporous crystals that are synthesized and reported every year, and considering also the hypothetical frameworks of different classes (*e.g.* zeolites, MOFs, COFs, ...), one ends up with a database containing more than one million materials.
In this context, computational molecular simulation is the only tool that allows to assess quantitatively (or at least qualitatively) the performance of each nanoporous framework for each application with the twofold aim of understanding the structure/properties relationships and find the best material for any specific application. To address these key issues we employ AiiDA, a python-based platform providing a common language for automating, sharing, updating and expanding the investigation of gas adsorption.

Poster 18

M. Sadowski, K. Albe

Modeling of Lithium Thiophosphates: Transport Properties and Interfacial (In)Stability

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A promising solid electrolyte material class for the facilitation of all-solid-state batteries are Lithium thiophosphates as high lithium ionic conductivities are observed for certain phases. However, the non-trivial relationships between composition, synthesis conditions, structure and properties are not fully understood.
Our aim is to shed light on this interesting class of materials using Density Functional Theory (DFT), especially focusing on defect thermodynamics, transport properties and interface phenomena.
We present two different methodologies to reveal transport properties in a) the superionic conductor Li_4PS_4I *[Solid State Ionics 319, p. 83-91 (2018)]* and b) the ionic insulator $Li_4P_2S_6$ *[Chem. Mater. 28 (23), p. 8764-8773 (2016)]*. The former relies on ab-initio molecular dynamics (AIMD) and the latter on a combination of defect thermodynamics and nudged elastic band (NEB) calculations. Additionally, we reveal the interfacial instability of $Li_4P_2S_6$ against Li metal by using thermodynamics, explicit interface models and highlight an alternative approach that only relies on defect thermodynamics *[Solid State Ionics 319, p. 53-60 (2018)]*.

Poster 19

A. Silva [1], D. Kramer [1], T. Polcar [1,2]

Understanding the phase behaviour of MoS_2-Ti compounds

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2 Czech Technical University in Prague

Recent studies have highlighted the remarkable graphene-like properties of transition metal dichalcogenides (TMDs) and how their chemical composition make them suitable for functionalization and wide range of applications *[1,2]*.
In particular, MoS_2-Ti composite coatings are known to yield excellent tribological results in industrial testing *[3]* and its tribological properties has been recently characterised by means of atomistic simulations *[4]*.
Despite the great interest and numerous applications of this material, an understating of its thermodynamically stable structure and phase diagram is lacking. In this work we makes a step in the direction of filling this knowledge gap.
In order to address the challenging task of determining the phase-stability of a new compound, we map energy landscapes obtained with DFT onto a cluster-expansion Hamiltonian and iteratively search for low energy orderings of the atoms inside the given host through Monte Carlo simulations.
This methodology allows us to explore the Ti-Mo-S phase space, identify stable configurations of the form $Ti_xMo_{1-x}S_2$, quantify miscibility gaps and competition with ternary oxides as function of temperature. Moreover we study the effect of dimensionality on the stability of the system by simulating both 3D bulk structures and isolated 2D layers.

[1] Nat. Chem. 5, 263 (2013)
[2] Nat. Nanotechnol. 7, 699 (2012)
[3] Surf. Coatings Technol. 228, 275 (2013)
[4] Inorg. Chem. 54, 5739 (2015)

Poster 20

Harish K. Singh [1*], Zeying Zhang [2], Ingo Opahle [1], Dominik Ohmer [1], Yugui Yao [2], and Hongbin Zhang [1*]

High-Throughput Screening of Magnetic Antiperovskites

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2 Beijing Key Laboratory of Nanophotonics and Ultrafine Optoelectronic Systems, School of Physics, Beijing Institute of Technology, Beijing 100081, China

Like perovskite materials, antiperovskites display many intriguing physical properties. In this work, we carried out high-throughput density functional theory calculations to evaluate the stability of magnetic antiperovskite compounds.
We screened 630 cubic antiperovskites M_3XZ (M = Cr, Mn, Fe, Co, and Ni; Z = C, N; and X is one of the elements from Li to Bi except noble gases and 4*f* rare-earth metals) in order to validate the experimentally known phases and to predict novel systems.
Thermodynamical, mechanical, and dynamical stabilities are considered, which are obtained by evaluating the formation energy with convex hull, elastic constants, and phonon dispersion, respectively. Eleven antiperovskites so far not reported in the ICSD database fulfill all the already mentioned stability criteria, suggesting that their synthesis as bulk phases is likely. A softening of the already-mentioned stability criteria results in more than 50 potentially new materials, where synthesis as thin film or in related structures may be possible. The chemical trends in the stability are analyzed on the basis of the crystal orbital Hamilton population.

Poster 21

J.R. Sucker , C. Roedl , J. Furthmueller, F. Bechstedt, S. Botti

Strain engineering of lonsdaleite germanium

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The design of CMOS integrable laser sources allows for intra- and inter-chip optical communications at an attojoule/bit energy consumption.
To this end, a pure silicon laser would be the ideal solution, but Si has an indirect band gap and, therefore, it is not suitable for laser applications.
Hexagonal Ge, on the other hand, may represent a viable alternative: It features excellent CMOS compatibility and, even though its direct gap of 0.3 eV is only weakly dipole allowed, the strongly dipole-active optical transition to the second conduction band is only about 0.3 eV higher in energy *[Phys. Rev. Materials 3, 034602 (2019)]*.
This opens the way to band-structure engineering by structural modifications, such as nanostructuring, alloying, or straining.
Here, we use *ab initio* density-functional theory to investigate the impact of lattice strains (hydrostatic pressure, biaxial strain, uniaxial strain, etc.) on the electronic structure of hexagonal Ge.
We demonstrate that the order of the two lowest conduction bands can be inverted with less than 2% of tensile uniaxial strain which strongly improves the light-emission properties of hexagonal Ge.

Poster 22

A. Togo and I. Tanaka

Automation of phonon calculations and making phonon database

Kyoto university

We performed 10000 first-principles phonon calculations and made a phonon calculation database (*http://phonondb.mtl.kyoto-u.ac.jp/*). We show the technical details on this work.

Poster 23

Lorenzo Varrassi

Optical properties of transition metal perovskites by BSE

University of Bologna

We study the optical properties of a representative set of transition metal perovskites (including 3*d*, 4*d* and 5*d* compounds) by solving the Bethe-Salpeter equation, where the quasi-particle energies and screened interaction *W* are obtained by the *GW* approximation.
We evaluate the role and contribution of the excitonic effect to the spectra of the various materials and the origin of structures in the spectra themselves. Moreover, agreement between the spectra and the experimentally available measurements is discussed, as well as the comparison with the *GW* spectra.
We also employ an alternative and computationally cheaper approach, based on a model dielectric function, and discuss its usefulness and results with respect to the BSE spectra.
We plan to incorporate the simulated spectra in a database, containing the proprieties of different sets of material calculated with beyond-DFT methods, which is currently under development at the University of Vienna.

Poster 24

Pezhman Zarabadi-Poor

High-Throughput Screening of MOFs for Helium Production from Natural Gas

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