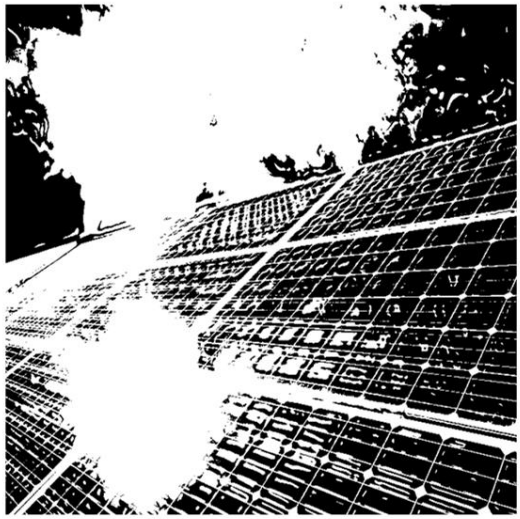


MCC+VASP WORKSHOP

London South Bank University

January 19th – 21st 2026

materials design

epcc

London South Bank University

EST 1892

UCL

Welcome

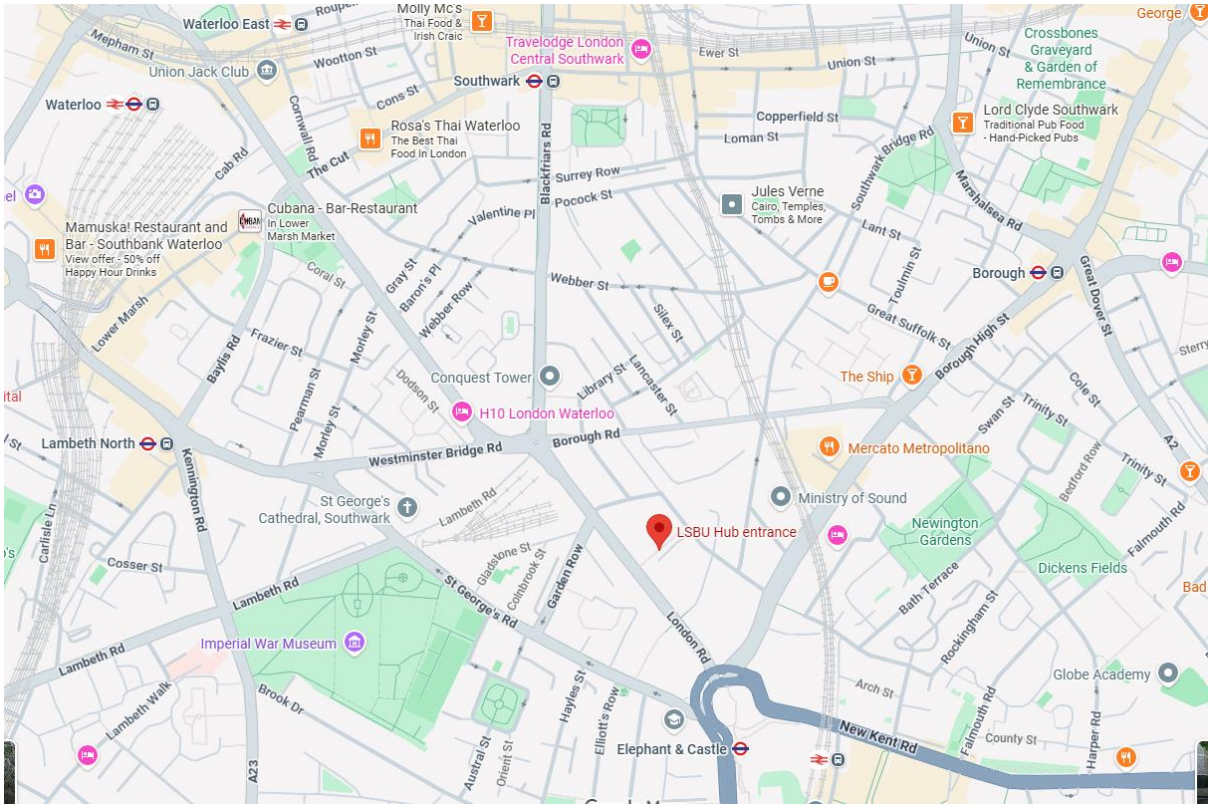
Welcome to the MCC+VASP workshop!

The workshop aims to help you learn about the features of VASP, discuss best practice, get the best performance from VASP on the ARCHER2 tier I supercomputer and to introduce you to the MedeA Software provided by Materials Design. You will have an opportunity to discuss your research and bring up all issues and problems you have encountered when running VASP, or that you envisage within the course of your research if you are a new user. We will have experts from Materials Design, from the VASP team and from EPCC partaking in the workshop and offering their assistance.

The Materials Design team will lead a hands-on session on Tuesday afternoon and will provide access to their software for a few weeks after the workshop.

Location/Maps

The workshop is taking place in the **LSBU Hub**, which is between the London Road and Keyworth Street (note the main entrance is *not* on Thomas Doyle Street, but on the next street south, see map below or follow link). Access via the main door. On registration, you will receive a guest pass from the security desk. The workshop will take place on the 2nd floor in the Waterloo Lecture theatre. Lunch and coffee breaks will be in the mezzanine outside the lecture theatres.



The nearest tube station is **Elephant and Castle** (**Bakerloo** and **Northern** lines). There is also an overground rail station there.
Other tube/train stations (10-15 min walk): Waterloo, Southwark, Borough, Lambeth North.
See here for more information on transport links.

Online Link and Internet/Wifi

The scheduled talks will be streamed using **MS Teams.** The link is as follows:

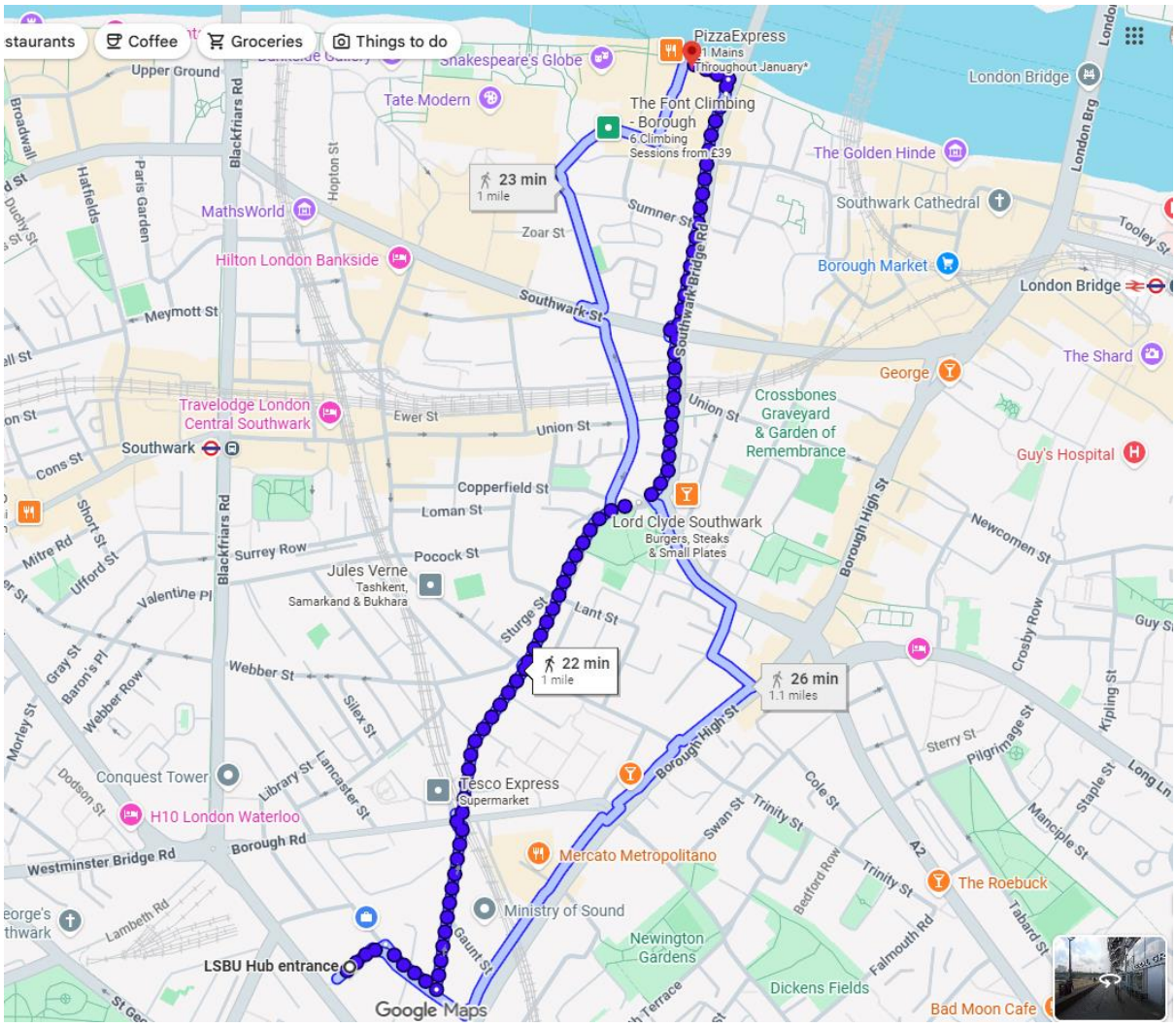
Microsoft Teams meeting
Join:

Wifi is available throughout the workshop space. You can connect to **Eduroam**, or there is the **LSBU Guest** wifi network. Please use the following credentials:

username: mccvasp
Password: QBF1E8PncC

Workshop Group Meal

We will have a group meal at 18:30 on Tuesday the 20th of January in the Real Greek, Bankside. It is about a 20 minute walk from the workshop location (see map below). Other options rather than walking would be to take the Northern Line from Elephant and Castle Underground Station to London Bridge, then walking from there (about a 5 minute walk), or taking an overground train from Elephant and Castle Rail Station to Blackfriars Station, and walking from there (also about 5 minutes).



Programme

Monday 19th January:

13:00-14:00 Registration (LSBU Hub Security Desk)

Session 1: Participants' Research Talks (Waterloo Lecture Theatre, floor 2 LSBU Hub)
Chair: John Buckeridge

14:00 **Welcome and Introduction** (John Buckeridge, LSBU)

14:10 **Effectiveness of Y, W, and Mo as *n*-type dopants in predicted TCO $Cd_2Sb_2O_7$**
Peter P. Russell, School of Chemistry, University of Birmingham

14:30 **Exploring Vacancy Formation in Ceria with Dispersion Corrections**
Thomas Hill, Department of Chemistry, Cardiff University

14:50 **Predicating the Defect Chemistry of Uranium Oxycarbide and the Accommodation of Xenon**
Reece Bedford, School of Engineering, Lancaster University

15:10 **Resonant Doping in Sb(V)-Based Oxides for High-Mobility Transparent Conducting Oxides**
Ke Li, Department of Chemistry, University College London

15:30 Tea, Coffee and Refreshments (floor 2 mezzanine)

16:00 **Revealing the lead phosphate system**
Victor Naden Robinson, Department of Chemistry, University of Nottingham

16:20 **Harnessing the potential of Halide Perovskites for Next-Generation Photocatalysis**
David J. Willock, Cardiff Catalysis Institute, School of Chemistry, Cardiff University

16:50 **Using dynamics to determine the ground state properties of g-C_3N_4**
Md Maruf Mridha, School of Engineering and Design, London South Bank University

17:10 **Computationally driven exploration of the structure and electronic properties of Cu_2GeSe_3 for use in high-performance thin film photovoltaic alloys**
Philippa U. Cox, School of Chemistry, University of Birmingham

17:30 **High-throughput and machine-learning-assisted design of high-performance ZnO-based piezoelectrics**
Aritra Roy, School of Engineering and Design, London South Bank University

17:50 Close

Tuesday 20th January:

Session 2: Meet the Experts (Waterloo Lecture Theatre, floor 2 LSBU Hub)
Chair: Brian Dron

09:30 **Auxilarly field quantum Monte-Carlo: recent advances and solids**
Georg Kresse, VASP Software GmbH

10:30 Tea, Coffee and Refreshments (floor 2 mezzanine)

11:00 **VASP performance and emissions efficiency**
Andy Turner, EPCC

11:30 **From femto to micro: bridging the length and time scales with MedeA**
David Reith and René Windiks, Materials Design

12:30 Lunch (floor 2 mezzanine)

Session 3: Meet the Experts cont'd
and Hands-On (Waterloo Lecture Theatre, floor 2 LSBU Hub)

13:30 **VASP 6.6.0 release: AMD / Intel GPU support via OMP target offload**
Michael Wolloch, VASP Software GmbH

14:30 **MedeA Hands-On**
David Reith and René Windiks, Materials Design

15:30 Tea, Coffee and Refreshments (floor 2 mezzanine)

16:00 ***Session continues***

17:30 Close

18:30 Workshop Meal (Real Greek, Bankside)

Wednesday 21st January:

Session 4: Outlook/Further Uses of VASP (Waterloo Lecture Theatre, floor 2 LSBU Hub)
Chair: Alexey Sokol

09:30 **Modelling the Phase Transition of $BiVO_4$ Using Machine-Learned Interatomic Potentials from Hybrid Functional and Random-Phase Approximation Data**
Taifeng Liu, Henan University

10:00 **Amide-Rich NaH as a Highly Active Catalyst for Ammonia Synthesis**
Michael D. Higham, School of Chemistry, Cardiff University

10:30 Tea, Coffee and Refreshments (floor 2 mezzanine)

11:00 **Nanoparticle synthesis, characterisation and functionalisation: challenges and outlook**
Suela Kellici, School of Engineering and Design, London South Bank University

11:20 **Designing materials for thorium nuclear clocks**
Harry W. T. Morgan, Department of Chemistry, University of Manchester

11:40 **Title TBC**
Speaker TBC, University of Exeter

12:00 **Challenges in computational materials chemistry and physics**
Richard Catlow, UCL, Cardiff University, Catalysis Hub

12:30 Close

Book of Abstracts

Effectiveness of Y, W, and Mo as *n*-type dopants in predicted TCO $Cd_2Sb_2O_7$

Peter P. Russell*,[1] Romain Claes,[1] Ke Li,[2] Alexander G. Squires,[1] and David O. Scanlon[1]

[1] *School of Chemistry, University of Birmingham,*
[2] *Department of Chemistry, University College London*

Transparent conducting oxides (TCOs) are central to the field of modern optoelectronics, displaying a unique combination of high electrical conductivity and optical transparency, with applications in touch screens, photovoltaics, and more.[1]

Recently, Sb(V) oxides have emerged as promising candidates.[2,3] Sb(V) possesses the $(n-1)d^{10}ns^0$ np^0 electron configuration common to many TCO cations, including In(III) in In_2O_3, leading to a highly disperse conduction band and a large band gap.[3] Furthermore, the Sb oxides have a greater diversity in band alignment compared to conventional TCOs, offering improvements in efficiency and the possibility of new device architectures. $ZnSb_2O_6$ [2] was computationally predicted and experimentally realised as a TCO, with other predicted candidates including $MgSb_2O_6$ and $CdSb_2O_6$, motivating further exploration of this family of materials.[4]

$Cd_2Sb_2O_7$ contains Sb(V) and was flagged in a high-throughput study as having a relatively large band gap and low electron effective mass, suggesting possible transparency and conductivity.[5] However, there had been no investigation into the material's defect chemistry. For these reasons it was decided to investigate $Cd_2Sb_2O_7$ more thoroughly. Our results predicted a degenerate intrinsic semiconductor with an optical gap in the transparent range and a large *n*-type doping window.

Further to this, we have investigated the possibility of resonant doping with Y on the Cd site and with W and Mo on the Sb site. Resonant doping is an approach to dopant selection that prevents hybridization between the dopant valence orbitals and the bulk electronic structure, thereby retaining the bulk's favourable electronic mobility. Y and W were able to offer improvements to carrier concentration over the intrinsic and achieve conductivity competitive with state-of-the-art TCOs. This provides further evidence for the potential of Sb(V) oxides as TCOs and the benefits of resonant doping in these materials.

[1] Lewis, B. G.; Paine, D. C. *MRS Bulletin* 2000, 25, 22
[2] Jackson, A. J.; Parrett, B. J. et al. *ACS Energy Letters* 2022, 7, 3807
[3] Li, K.; Willis, J. et al. *Chemistry of Materials* 2024, 36, 2907
[4] Claes, R.; Li, K.; et. Al. *ChemRxiv* 2025, 10.26434/chemrxiv-2025-39bbf
[5] Hautier, G.; Miglio, A.; et al. *Chemistry of Materials* 2014, 26 (19), 5447

Exploring Vacancy Formation in Ceria with Dispersion Corrections

Thomas Hill*, Igor Kowalec, C. Richard A. Catlow

[*]Department of Chemistry, Cardiff University

Computational modelling of metal oxides plays a crucial role in understanding the roles they play in catalysis, being both a support and an active catalyst.[1] Ceria is well known for its oxygen storage capacity which is facilitated by the variable valence cerium atom allowing rapid formation and healing of oxygen vacancies.[1]

Modelling of these systems can be problematic due to the highly correlated nature of the electrons in *d* and *f* orbitals. Descriptions of highly correlated systems like ceria and wrongly described by KS-DFT, showing strong delocalisation of electrons.[2] In standard KS-DFT corrections to the pseudopotential can be made to more accurately describe experimental data, these include the Hubbard U correction and Grimme's D3 dispersion correction.[1] Hybrid functionals provide much more accurate description of metal oxides but come at a great computational cost.[3] A systematic comparison of these methods was carried out to determine if the corrections could reproduce data that a higher level of theory is capable of.

All calculations were carried out in VASP.[4] The GGA PBE functional was used alongside the Dudarev Hubbard U and Grimme's D3 dispersion correction.[5] The projector augmented wave formalism was used to describe core electrons, and the Monkhorst-pack grid was used to sample the Brillouin zone.

[1] J. Paier, C. Penschke and J. Sauer, *Chem Rev*, 2013, 113, 3949.
[2] J. P. Allen and G. W. Watson, *Physical Chemistry Chemical Physics*, 2014, 16, 21016.
[3] D. Du, M. J. Wolf, K. Hermansson and P. Broqvist, *Phys Rev B*, 2018, 97, 235203.
[4] G. Kresse and J. Furthmüller, *Comput Mater Sci*, 1996, 6, 15.
[5] S. Grimme, *J Comput Chem*, 2006, 27, 1787.

Predicating the Defect Chemistry of Uranium Oxycarbide and the Accommodation of Xenon

Reece Bedford*[1], Sophie Cooper[2], Llyod Jones[2], Samuel Murphy[1]

[1] *School of Engineering, Lancaster University*
[2] *United Kingdom National Nuclear Laboratory, Warrington*

Tri-structural isotropic particle fuels (TRISO) are a current subject of interest for the use in Generation IV high-temperature nuclear reactors. The particles consist of an inner fuel kernel, wrapped in layers of mixed carbon-and-ceramic materials. This possesses several advantages over conventional fuel designs, such as increased temperature resistance, greater structural integrity and a self-containment system for fission products.

The inner fuel kernel has the potential to take on many forms, but using traditional uranium dioxide (UO2) was found to have significant safety concerns due to the evolution of carbon monoxide (CO). The formation of CO can be mitigated by introducing uranium carbide (UCx) into the fuel matrix, forming uranium oxycarbide (UCO). However, the chemistry of UCO is complex, and it is not well understood how the properties of UCO in a reactor differ from pure UO2. Particularly, understanding the mechanisms of fission gas behaviour is paramount for the performance of a fuel. It is currently assumed that such properties of UCO are the same as in UO2, however, there is significant degree of uncertainty around this.

Therefore, this work will combine Density Functional Theory (DFT) with thermodynamics to predict the intrinsic defect chemistry of UCO. From this, the uptake of carbon in the UO2 phases, and the propensity of UCx to be oxidised (i.e.: remove excess oxygen gas) can be modelled. Then, Xenon (Xe) defects will be introduced to determine and the preferred trap sites in UCO will be determined.

Resonant Doping in Sb(V)-Based Oxides for High-Mobility Transparent Conducting Oxides

Ke Li,[1] Romain Claes,[2] Alexander G. Squires,[2] David O. Scanlon[2]

[1]Department of Chemistry, University College London
[2]School of Chemistry, University of Birmingham

Transparent conducting oxides (TCOs) combine high conductivity with optical transparency, underpinning a wide range of optoelectronic technologies. $ZnSb_2O_6$ and Sb_2O^5 were recently realized and predicted as an earth-abundant TCO with Ga and F doping.1,2 Resonant dopants are attractive for TCO applications as their donor d-states sit well above the conduction band minimum, preserving high mobility while enabling high carrier concentrations.

In this work, we employ PBE0 functional density functional theory to investigate the resonant doping behaviour of Sc in $ZnSb_2O_6$ and of Mo and W in Sb_2O_5 and $ZnSb_2O_6$.[2,3] Both materials have wide n-type doping windows, which are optimal for extrinsic dopants incorporation. In $ZnSb_2O_6$, Sc acts as a resonant dopant, with the unfolded band structure showing its 3d states positioned ~ 4.5 eV above the conduction band edge. This preserves the dispersive Sb 5s at CBM and yields an overall electron concentration of 10^{19} – 10^{20} cm^{-3}, showing n-type degenerate transparent conducting oxide behaviour. Mo and W were chosen as potential candidates to substitute the Sb site for both materials, based on the success of Mo doping in In_2O_3 and W doping in SnO_2.[4,5] Although the substitution defects residing in the bandgap for Mo- and W-doped $ZnSb_2O_6$, they incorporate favourably in Sb_2O_5, where both substitution defects exhibit low formation energies and have localised d-states appearing above the CBM. These findings broaden the design principles for optimization of Sb(V)-based transparent conductors.

[1] Jackson, A. J, et al., *ACS Energy Lett*., 2022, **7**, 3807-3816.
[2] Li, K. et al., *Chem. Mater*., 2024, **36**, 2907-2916.
[3] Adamo, C.et al.;. *J. Chem., Phys.,* 1999, **110**, 6158–6170.
[4] Swallow, J., et al., *Mater. Horiz.,* 2020, **7**, 236.
[5] Fukumoto, M.et al., *Adv. Funct. Mater.,* 2022, **32**, 2110832.

Revealing the lead phosphate system

Victor Naden Robinson*, Shayantan Chaudhuri, John Vinson, Katherine Inzan

[*]Department of Chemistry, University of Nottingham

We present *ab initio* calculations on the Pb–PO_4 system, which is important in ceramics and glasses, revealing the energetic ranking of experimentally known phases. We investigate exchange–correlation functional dependence, phase relations and transitions, and search for new phases via crystal structure prediction. We find that the ground state structure for $Pb_3(PO_4)_2$ is a rarely observed C2/c structure (we name ɣ), as opposed to another C2/c structure (α) commonly found at room temperature. $Pb_3(PO_4)_2$ is also observed to have a ferroelectric phase transition between α and an $R\bar{3}m$ phase (β). Structure searching results for the $Pb_3(PO_4)_2$ composition confirm that these are the lowest energy phases. Interestingly, the α phase was found more often than the rarely observed ɣ phase, which was only found once, similar to its experimental occurrence. Compressing this system to moderate pressures can lead to phase transitions and naturally joins some of these related phases.

Harnessing the potential of Halide Perovskites for Next-Generation Photocatalysis

David J. Willock*

** Cardiff Catalysis Institute, School of Chemistry, Cardiff University*

Metal halide perovskites have emerged as semi-conducting materials with great promise for photovoltaic power generation. The ABX_3 formulation, with A a mono-valent cation B a divalent cation and X a halogen allows tuning of the band gap and band edge positions. However, these materials have drawbacks in terms of toxicity concerns, when B=Pb and stability concerns, particularly if exposed to water. In this work we have used density functional theory to compare materials with B=Pb and Sn, as a possible alternative with lower toxicity. The thermodynamic stability is considered using ab inito derived phase diagrams for bulk cubic and orthorhombic structure and for their surfaces. The band structure is analysed at a range of levels, and we show that the HSE06 level ($\alpha = 0.5$) with SOC for Pb gives good agreement with the available experimental data. We then consider stabilising 2-D halide perovskites using organic ligands to cap surface sites.

Using dynamics to determine the ground state properties of g-C_3N_4

Md Maruf Mridha*, Suella Kellici, and John Buckeridge

*School of Engineering and Design, London South Bank University

Graphitic carbon nitride (g-C_3N_4) is a promising photocatalyst with unique structural, electronic and thermodynamic properties that at present requires a favourable semiconducting co-catalyst for efficient water splitting performance due to its poor charge mobility and fast photogenerated charge recombination. g-C_3N_4 may exist in three phases, but there are many outstanding questions regarding its ground state properties. Here, we perform a thorough investigation of the ground state structural and electronic properties of all three phases of g-C_3N_4, including bulk and single layer systems, using a range of density functional theory approaches. By investigating second order phase transitions, we determine the dynamically stable ground state configurations of each phase, finding that the system will 'buckle' substantially even in the bulk phases, and that this buckling or corrugation occurs within moieties, not just among them. We find that the fundamental band gap varies by over 2 eV, depending on structure. Moreover, the bulk and surface energetics indicate that real samples may contain multiple phases and structures, and that the measured band gap is most likely an average value. We also compute band alignments with regards to the redox potential lines that vary strongly with structure and which indicate that preferential buckling may be beneficial for photocatalytic water splitting. Finally, analysis of the charge distributions of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) suggests that buckled structures may offer more favourable water oxidation and reduction sites, although for efficient activity co-catalysts will be required. Our study provides key information on this important material that may help the design of efficient photocatalysts for H_2 production.

Computationally driven exploration of the structure and electronic properties of Cu2GeSe3 for use in high-performance thin film photovoltaic alloys.

Philippa U. Cox, Alexander G. Squires, Peter P. Russell, Romain Claes, David O. Scanlon

* *School of chemistry, University of Birmingham*

Ternary diamond-like copper chalcogenides are amongst the highest performing single-junction thin film photovoltaic materials[1]. They exhibit lower toxicity and greater stability than CdTe and perovskite single-junction photovoltaics, while maintaining high performance at reduced film thicknesses relative to silicon[2]. The highest performer Cu(In,Ga)Se2 has reached a record power conversion efficiency of 23.6% at thicknesses lower than 2.0μm[3]. However, industry applications are limited due to the high cost of scarce elements and the precise synthesis required to minimize performance-reducing defects[4]. Copper zinc tin selenide was developed in an attempt to produce a low-cost high-performance thin film material, but performance has stalled at 15.8% due to high concentrations of charge recombination centres[5]. As a result, developing new thin film photovoltaic materials remains an important area of research.

Cu_2GeSe_3 has been explored as a thermoelectric for many years, it contains a larger proportion of cheap, non-toxic and abundant materials than CIGS, with good thermal and chemical stability[6]. Previous work by the Scanlon Materials Theory Group has identified the silicon analogue Cu_2GeSe_3 as a promising defect tolerant photovoltaic material with a high theoretical power conversion efficiency of 30%[7]. Despite its narrower optical band gap of 0.78-0.85 eV, the germanium system may offer promising properties as a bottom layer for tandem cells, dopant or alloy in photovoltaic thin films[8]. However, little is known about the structure and properties of Cu_2GeSe_3. Once believed to be ordered, Cu_2GeSe_3 has now been shown to be more complex[9]. It is essential to comprehensively characterise Cu_2GeSe_3 to ensure its suitability as a photovoltaic material.

This work aims to explore the structure and properties of Cu_2GeSe_3 for use in photovoltaic alloys by employing a combined density functional theory, machine learning approach. Our approach uses machine learning interatomic potentials to calculate the vibrational free energies of a range of structures for use in cluster expansions for Monte Carlo simulation-based disorder studies.

[1] Sivasankar, S.M., et al., A.F.D., 2025. *J. Composites Sci.*, 9(3), 143.
[2] Sajitha, D.R., et al., 2024. *Prog Solid St. Chem.*, 76, 100490.
[3] Green, M.A., et al., 2024. Solar cell efficiency tables (Version 64). *Progress in photovoltaics: research and applications*, *32*(7), 425.
[4] Brammertz, G., et al., 2025. *ACS Applied Materials & Interfaces*, 17(33), 46998.
[5] Shah, U.A., et al., 2024. *Small*, 20(30), 2310584.
[6] Cho, J.Y., et al., 2011. *Phys. Rev. B*, 84(8), 085207.
[7] Nicolson, A., et al., 2023. *J. Mater. Chem. A*, 11(27), 14833.
[8] Chetty, R., et al., *Intermetallics*, 2014, 54, 1.
[9] Dugarte-Dugarte, A., et al., 2021. *Structural Science*, 77(1), 158.

High-throughput and machine-learning-assisted design of high-performance ZnO-based piezoelectrics

Aritra Roy*, Enrico Grisan, Chiara Gattinoni, John Buckeridge

Energy, Materials and Environment Research Centre, London South Bank University

Piezoelectric materials have wide applicability in many modern sensor devices. Improving such devices requires the design of materials with high electrical responses to mechanical strain. Polar systems in the wurtzite phase tend to display piezoelectricity, a key example being the abundant metal oxide ZnO. However, its piezoelectric strain coefficient (d_{33}) of ~12 pC/N[1] is about 30 times lower than composites based on oxide perovskites such as $BaTiO_3$. Such composites tend to include the toxic element Pb. Doping or alloying ZnO with other metal oxides or piezoelectric compounds could increase the piezoelectric coefficient sufficiently to make the system competitive with other oxides for devices. Hence, we aimed to develop a high-throughput electronic structure calculations framework based on VASP[2] to search the space spanned by a range of ZnO-based system of alloys $A_xB_yZn_{1-x-y}C_zO_{1-z}$ where C = S^{2-} or Se^{2-}, and A, B can be Mg^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Cd^{2+}, Hg^{2+}, Na^{+}, K^{+}, Cs^{+}, Al^{3+}, Ga^{3+}, Y^{3+}. But the compositions that can be computed efficiently is quite limited in terms of the total possible structures. Deep learning algorithms can be trained on such calculations and employed to predict piezoelectric properties for a broader range of compositions.

To generate the data for the DL model, we developed DopantFlow, an in-house high-throughput framework based on VASP to carry out a series of computations (relaxation and piezoelectric calculations) for each supercell with varying compositions of metal and anion dopants. All computations employ plane-wave density functional theory (DFT) using the PBEsol functional,[3] which provide sufficient accuracy while ensuring the calculations are tractable. Till now ~1500 doped structures have been calculated using DopantFlow which will be used to train a deep learning model to predict new composition which will have higher piezoelectric strain coefficient.

[1] Catti et al., *J. Phys. Chem. Sol.* 64, 2183 (2003)
[2] Kresse et al., *Phys. Rev. B.* 54, 11169 (1996)
[3] Perdew et al., *Phys. Rev. Lett.* 100, 136406 (2008)

VASP performance and emissions efficiency

Andy Turner*

[*]EPCC, Edinburgh

In this presentation we will provide data on VASP performance on a selection of CPU and GPU national HPC services based at EPCC and present some guidance on how to choose compile options and parameters to optimise VASP performance on these types of architectures. As well as performance, we will present an evaluation of the emissions efficiency of VASP across systems and parameter choice and provide a summary of how to try and minimise carbon emissions from running VASP on large scale HPC systems.

Modelling the Phase Transition of $BiVO_4$ Using Machine-Learned Interatomic Potentials from Hybrid Functional and Random-Phase Approximation Data

Taifeng Liu*

* *National & Local Joint Engineering Research Center for Applied Technology of Hybrid Nanomaterials, Henan University,*

$BiVO_4$ is a key photocatalytic and ferroelastic material. Conventional density functional theory (DFT) with standard exchange-correlation functionals fails to accurately describe its monoclinic-to-tetragonal phase transition, as they incorrectly predict a low-symmetry structure and lack the soft modes observed in high-symmetry structure experimentally. While hybrid functionals with high exact-exchange mixing (~60%) correct this, they are computationally prohibitive for large-scale simulations. To overcome this, we train machine-learned interatomic potentials (MLIPs) using data from high-accuracy hybrid functional calculations. The developed MACE-MP-0-based potentials successfully reproduce hybrid DFT results at a fraction of the cost. Furthermore, to move beyond system-specific hybrid parameters, we employ the parameter-free random-phase approximation (RPA) to generate additional training data. We compare MLIPs trained from hybrid DFT and RPA, providing a robust framework for simulating soft-mode-driven phase transitions in ABO_4 and related materials.

Amide-Rich NaH as a Highly Active Catalyst for Ammonia Synthesis

Michael D. Higham*, Matthew S. Cummings, William I. F. David, C. Richard A. Catlow

School of Chemistry, Cardiff University

Ammonia synthesis is also one of the most environmentally challenging industrial processes, with ammonia production being responsible for an estimated 1.8% of global energy consumption. Recent experimental studies have revealed that the $NaNH_2$ catalyst is highly active for ammonia cracking, and may also be a highly active catalyst for ammonia production. It is believed that the active phase resembles a NH_2-rich sodium hydride phase. Hence, in the present work, DFT techniques are applied to model the proposed active phase, and investigate surface reaction processes to determine the likely reaction mechanism. In the present work, plane-wave DFT calculations using the VASP code. In order to approximate the predominant active phase identified from the experimental results, a model was constructed based on a NaH(100) (2x2) surface facet with NH_2 amide species substituting a fraction of lattice hydride, in order to represent an amide-rich hydride phase. The PBE exchange-correlation functional with a D3 dispersion correction (with Becke-Johnson damping) was applied, along with a 600 eV plane-wave cut-off energy; k-point sampling with performed using a 6x6x1 Monkhorst-Pack grid. Geometric optimization was performed until forces were converged to within 0.01 eVÅ-1. Transition states were obtained using the Nudged Elastic Band (NEB method) and dimer methods. The calculations reveal that surface hydride/amide vacancies can facilitate N_2 activation, with N_2 adsorbing exothermically with elongation of the N-N bond. Whilst hydrogenation of N_2 requires adjacent H/NH_2 vacancies, dissociation of intermediates such as $NHNH_2$ is facile. NH is readily hydrogenated to regenerate NH_2, the NH_2 species is highly stable, and its hydrogenation to yield ammonia is highly energy demanding. The calculations demonstrate how H/NH_2 vacancies on the NaH(100) surface can facilitate ammonia synthesis via a Mars-van-Krevelen type mechanism.

Designing materials for thorium nuclear clocks

Harry W. T. Morgan*

Department of Chemistry, University of Manchester

The ^{229}Th isotope has a nuclear excited state at 8.4 eV above the ground state that can be excited with a tabletop laser, as demonstrated for the first time in 2024 after a 50-year search.[1,2] The frequency of this transition is extremely well defined and, being a purely nuclear process, insensitive to environmental perturbations. It therefore holds great potential as a next-generation clock, outperforming atomic clocks by orders of magnitude. A major goal is development of a solid-state nuclear clock, where ^{229}Th is present in a host material rather than an optical trap.[3] A solid-state clock would have a high concentration of ^{229}Th nuclei, allowing us to reach high accuracy in rapid measurements, and it would be chemically and physically durable, making it suitable for applications from millimetre-accurate GPS to earthquake prediction.

The properties of the device will be determined by the host material, so rational material design is essential. We have used VASP calculations to compute structural, electronic, and optical properties of stoichiometric thorium compounds and thorium dopants.[4,5,6] In this talk I will present the story of ^{229}Th from a chemist's perspective, describe current challenges, and highlight the role that computational materials chemistry can play in this exciting new field.

[1] *Physical Review Letters* 133, 1, 013201 (2024)
[2] *Physical Review Letters* 132, 18, 182501 (2024)
[3] *Nature* 636, 8043, 603 (2024)
[4] *Applied Physics Letters* 126, 111101 (2025)
[5] *Dalton Transactions* 54,10574 (2025)
[6] *Nature* 648, 300 (2025)