WORKSHOP REPORT

http://www.imperial.ac.uk/mssc2018/

Abstract

The Department of Chemistry and the Thomas Young Centre at Imperial College London and the Computational Materials Science Group of the Science and Technology Facilities Council (STFC), in collaboration with the Theoretical Chemistry Group of the University of Torino, organised the 2018 MSSC Summer School on the "*ab initio* modelling of crystalline and defective solids with the CRYSTAL code".

CRYSTAL is a general-purpose program for the study of periodic solids. It uses a local basis set comprised of Gaussian type functions and can be used to perform calculations at the Hartree-Fock, density functional or global and range-separated hybrid functionals (e.g. B3LYP, HSE06), double hybrid levels of theory. Analytical first derivatives with respect to the nuclear coordinates and cell parameters and analytical derivatives, up to fourth order, with respect to an applied electric field (CPHF/CPKS) are available.

The school provided an overview of the underlying theory and fundamental issues affecting use of the code, with particular emphasis on practical issues in obtaining reliable data efficiently using modern computer hardware.

The capabilities of CRYSTAL was illustrated with hands-on tutorials organized in the afternoon sessions.

All information about the school can be found on this website:
http://www.imperial.ac.uk/mssc2018/

Attendees

Speakers

- Ehsan Ahmad - Imperial College London (UK)
- Maria L. Alfredsson - University of Kent (UK)
- Leonardo Bernasconi - STFC Rutherford Appleton Laboratory, Oxfordshire (UK)
- Gerit Brandenburg- University of Goettingen (Germany)/UCL (UK)
- Ian J. Bush - Oxford e-Research Centre, University of Oxford (UK)
- Silvia Casassa - Università di Torino (Italy)
- Furio Corà - University College London (UK)
- Atreyi Dasmahapatra - Università di Torino (Italy)
- Alessandro Erba - Università di Torino (Italy)
- Anna Ferrari - Università di Torino (Italy)
- Andrea Ferretti - S3 Center, Istituto Nanoscienze, CNR, Modena (Italy)
- Nic M. Harrison - Imperial College London (UK)
- Giuseppe Mallia - Imperial College London (UK)
- Ruth Martínez - Università di Torino (Torino)
- Lorenzo Maschio - Università di Torino (Torino)
- Barry G. Searle - STFC Daresbury Laboratory (UK)

Delegates

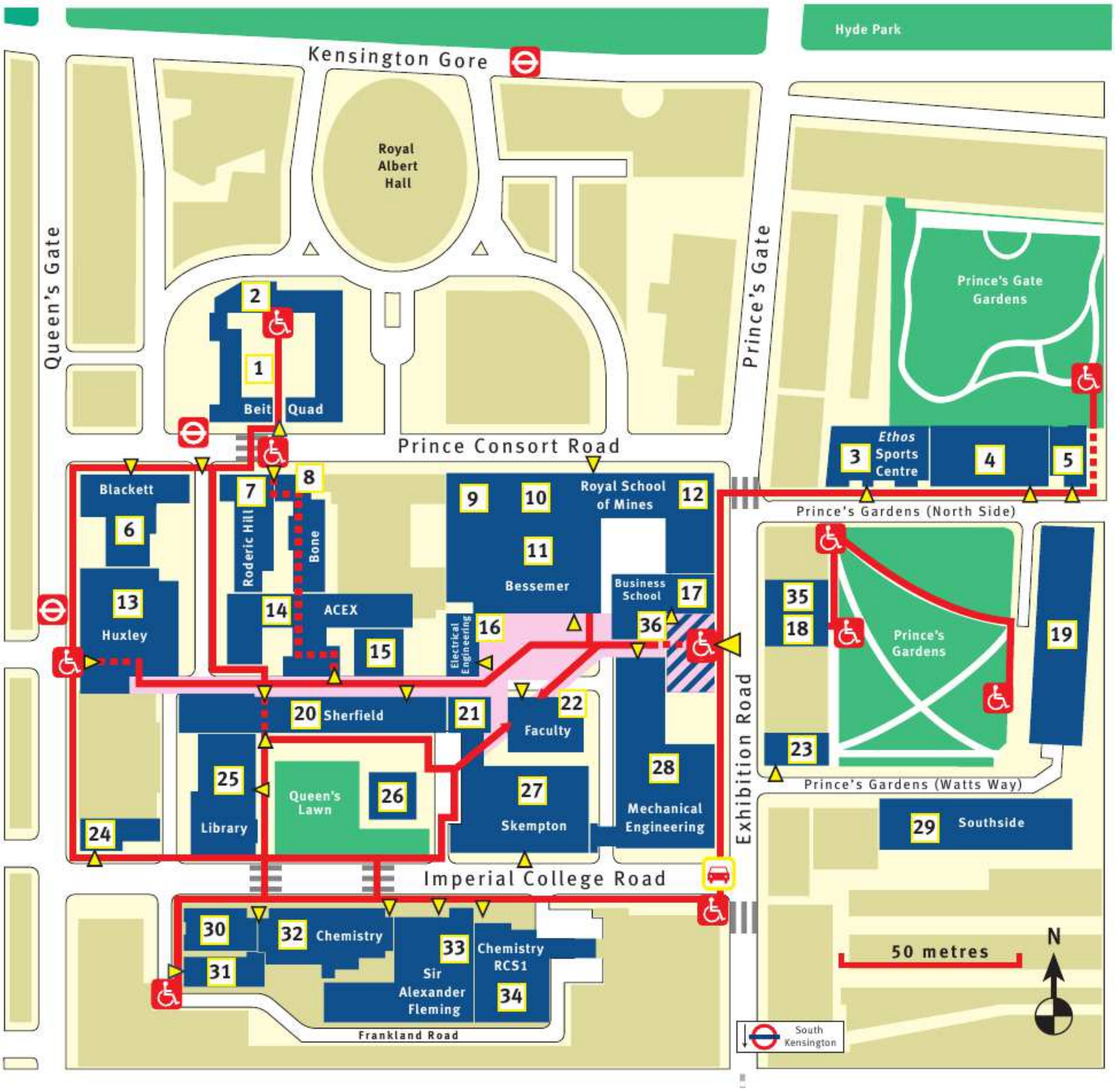
Title	First name(s)	Surname	Email
Dr	Benmakhlouf	Abdennour	a.benmakhlouf@lagh-univ.dz
Ms	Zainab	Alaithan	z.alaithan17@imperial.ac.uk
Mr	Rihards	Aleksis	rihards.aleksis@mmk.su.se
Mrs	Tahani	Almutairi	ta16535@bristol.ac.uk
Mr	Jasper	Berry-Gair	Jasper.berry.14@ucl.ac.uk
Mr	Prabal Dev	Bhuyan	prabal.bhuyan@sxca.edu.in
Mr	Shantonio	Birch	swbirch@umich.edu
Mr	David	Bowskill	david.bowskill13@imperial.ac.uk
Mr	José	Carvalho	jose.carvalho@mmk.su.se
Mr	Mohamed	Eldeeb	m.s.eldeeb@ifw-dresden.de
Dr	boutaiba	farouk	boutaiba_f@yahoo.fr
Dr	Jovanny	Gomez	jovanny.gomez@uptc.edu.co
Mr	Kyle	Groden	kyle.groden@wsu.edu
Mr	Liam	Harnett	liamharnett@hotmail.co.uk
Dr	Safia	IZZAOUIHDA	safiafssm@gmail.com
Mr	Stefanos	Konstantinopoulos	s.konstantinopoulos17@imperial.ac.uk
Miss	Guoda	Liepuoniute	gl4517@ic.ac.uk
Ms	Ieva	Liepuoniute	ieva@chem.ucla.edu
Mr	Zimen	Makwana	zimen.makwana14@imperial.ac.uk
Miss	Asmaa	MARCHOUD	marchoud.asmaa@gmail.com
Mr	Jorge Diogo	Marques Laranjeira	jorgelaranjeira@ua.pt
Dr	Liliana	Mazur	lmazur2@op.pl
Mr	Arpit	Mishra	arpit.mishra@edf.fr
Dr	Thai Thu Hien	Nguyen	h.nguyen1@leeds.ac.uk
Mr	Titas	Pramanik	titasiisc@gmail.com
Mr	Bartlomiej	Rzeszotarski	Rzeszotarski.bartek@gmail.com
Dr	Pralok	Samanta	pralok.samanta@ucd.ie
Mr	Aamir	Shafique	aamrshafique@gmail.com
Dr	Justyna	Sienkiewicz-Gromiuk	j.sienkiewicz-gromiuk@poczta.umcs.lublin.pl
Miss	Aliki Marina	Tsopelakou	a.tsopelakou16@imperial.ac.uk
Mr	Hamid	Ullah	hamid12@mail.ulsan.ac.kr
Mr	Garlef	Wartner	garlef.wartner@helmholtz-berlin.de
Dr	Jiayue	Yang	yang@ghi.rwth-aachen.de
Miss	Asmaa	ZARAQ	assmaa.zaraq@gmail.com
Miss	Xuewei	Zhang	xz5016@ic.ac.uk
Mr	Aleksandar	Živković	ZivkovicA@cardiff.ac.uk

Location

MSSC2018 took place from Monday 17 – Friday 21 September at...

- **Registrations and Morning Sessions - Royal School Of Mines, Prince Consort Rd, Kensington, London SW7 2BP (Building 12)**

- **Afternoon Sessions - Department of Chemistry/Biochemistry, South Kensington Campus, London SW7 2AZ (Building 32)**



Programme

MORNING SESSIONS:RSM - Room 1.31

Coffee Break: Royal School of Mines (RSM) / Department of Materials - Room 1.31

	Monday 17th	**Tuesday 18th**	**Wednesday 19th**	**Thursday 20th**	**Friday 21st**
9:00 - 9:45	Quantum Chemical Methods ***L. Bernasconi***	The structure of the CRYSTAL code ***G. Mallia***	One-electron properties ***F. Corà***	Localized crystalline orbitals and related quantities ***L. Bernasconi***	Dielectric and optical properties of solids ***L. Bernasconi***
9:45 - 10:30	Density-functional theory ***L. Bernasconi***	Modeling low-dimensional systems with CRYSTAL: Surfaces, Nanotubes and Fullerenes ***A. Ferrari***	Vibrational frequencies calculation and tools for their analysis ***A. Ferrari***	Post-HF techniques and the CRYSCOR project ***L. Maschio***	Excited states. TD-DFT ***L. Bernasconi***
	Coffee Break	*Coffee Break*	*Coffee Break*	*Coffee Break*	*Coffee Break*
10:50 - 11:35	How to Model Crystals: Periodic Boundary Conditions ***S. Casassa***	Local defects in crystalline materials ***G. Mallia***	Quasi-harmonic Approximation: Thermal Effects on Structural and Thermodynamic Properties ***A. Erba***	CRYSCOR: studied cases ***R. Martinez-Casado***	Ab initio transport properties and thermoelectric materials ***A. Dasmahapatra***
11:35 - 12:20	Geometry optimisation of solids ***A. Erba***	TOPOND: topological analysis of the electron charge density of solids ***S. Casassa***	Infrared and Raman Spectra of Solids ***L. Maschio***	Van der Waals interactions in the DFT framework ***G. Brandenburg***	Quantum transport in nanojunctions ***A. Ferretti***
12:20 - 13:05	CRYSTAL input/output. Basic features. Scripts. ***G. Mallia***	The effect of pressure: equations of state; bulk modulus; elastic constants **M. Alfredsson**	Ab initio thermodynamics **E. Ahmad**	CRYSTAL in parallel ***I. Bush***	Predictive simulation and materials characterisation ***N. Harrison***

AFTERNOON SESSIONS: Chemistry/Biochemistry Building

Coffee Break and Poster Session: Department of Chemistry
Chemistry Cafe' (Room 232)

BASIC TUTORIALS : ROOM 311 – BIOCHEMISTRY BUILDING

	Monday 17th	Tuesday 18th	Wednesday 19th	Thursday 20th	Friday 21st
14:30 - 16:15	Geometry input	DLV: visulisation of structures and properties. ***B. Searle*** Total energy (Single-point)	13:05 - 15:45 *Lunch* & *Poster Session*	Vibrational frequencies	Nanotube systems
	Coffee Break	*Coffee Break*		*Coffee Break*	*Coffee Break*
16:45 - 18:30	Basis set input & basis set editing	Geometry optimisation	16:00 ... *Self-guided Tour*	One-electron properties. TOPOND: electon densisty analysis	Basic modelling of surfaces and defects

ADVANCED TUTORIALS : ROOM 310 – BIOCHEMISTRY BUILDING

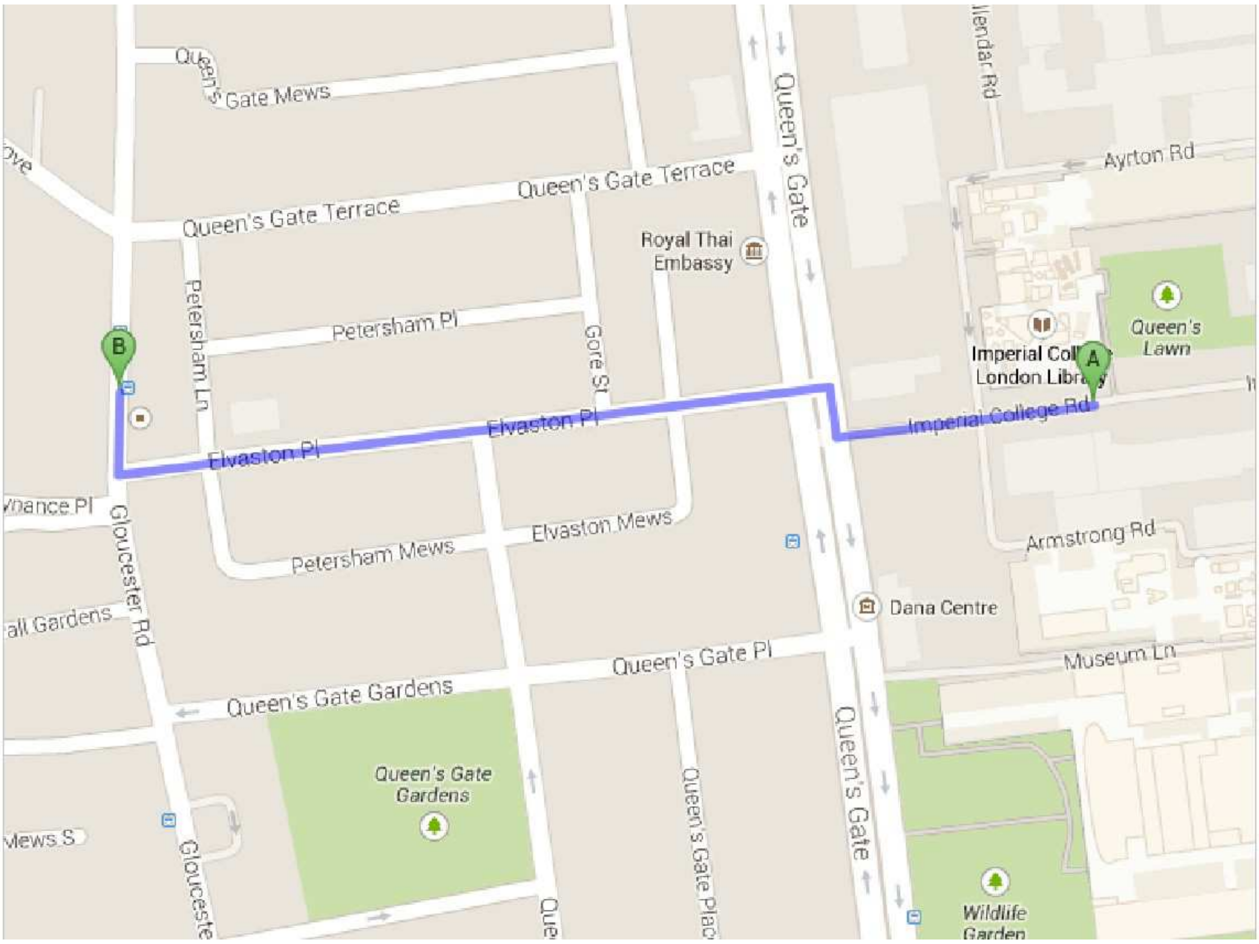
	Monday 17th	Tuesday 18th	Wednesday 19th	Thursday 20th	Friday 21st
14:30 - 16:15	Advanced options in geometry optimisation and frequencies calculation	Magnetic properties	13:05 - 15:45 *Lunch* & *Poster Session*	CRYSTAL in Parallel Mode: Pcrystal vs. MPPcrystal	Dielectric properties
	Coffee Break	*Coffee Break*		*Coffee Break*	*Coffee Break*
16:45 - 18:30	Advanced options in geometry optimisation and frequencies calculation	Magnetic properties	16:00 ... *Self-guided Tour*	CRYSCOR	Dielectric properties

Social Dinner

The MSSC Dinner took place on Wednesday 19 September at...

MED KITCHEN RESTAURAN
25–35 Gloucester Road
London SW7 4PL

The feedback about the dinner was very positive and attendees enjoyed the social interaction and to know each other.


A
B
Queen's Gate Mews
Queen's Gate Terrace
Queen's Gate
Royal Thai Embassy
Petersham Pl
Petersham Ln
Gore St
Elvaston Pl
Imperial College Rd
Imperial College London Library
Queen's Lawn
Ayrton Rd
Armstrong Rd
Dana Centre
Museum Ln
Elvaston Mews
Petersham Mews
Gloucester Rd
Queen's Gate Pl
Queen's Gate Gardens
Queen's Gate Place
Wildlife Garden

Poster Titles and Abstracts

Structural and Electronic properties of Graphene upon Hydrogen adsorption, a Quantum Mechanical study

Zimen Makwana, Mariana Hildebrand, Giuseppe Mallia, Nicholas M. Harrison

Inducing and tuning a chemical band-gap in graphene has generated much research interest in the physical and chemical adsorption of small molecules to its surface, as method for potential electronic applications. Here, periodic molecular hydrogen physisorption to graphene with differing coverages is presented. Structural effects on the graphene surface are dependent on both the coverage and adsorption geometry of H2. Electronic results suggest that H2 is a p-type dopant and can induce band-gaps upon adsorption. Varying coverages and geometries of H2 therefore presents a method to tune the band-gap of graphene via physiorption.

Energetics and Rotational Dynamics of Ligand Controlled Dirhodium-Centered Four-Gear Systems

Ieva Liepuoniute

The group of Mitsuhiko Shionoya from University of Tokyo has reported rotational control of a lantern-type dirhodium complexes with circularly arranged triptycene molecules used as a three-bladed gear, and two axial ligands utilized as rate control elements. Six different rotator systems were synthesized with axial ligands such as pyridine (py), 2-methylpyridine (mepy), 2-ethylpyridine (etpy), N,N-dimethyl-4-aminopyridine (damp), methyl isonicotinate (min), and ether. The results showed that rotational rates in solution were markedly affected by coordination ability and the bulkiness of axial ligands. Single crystal XRD revealed information about rotator structure, while solution state NMR studies allowed to calculate rotational parameters for all molecular gears except py, damp and min ligand systems. We performed molecular dynamics simulations using AMBER force field to further investigate the rotational motion and obtain energy parameters for all ligand systems. Calculations were performed in solution and in gas state, gaining an additional insight into rotational dynamics in a solvent free environment. This study expands our current knowledge on ligand exchange-based control of rotational motion and contributes to advancing stimulus-responsive metallo-molecular multirotors.

Heisenberg-Kitaev interactions in iridium oxides

Mohamed Eldeeb

Highly anisotropic magnetic couplings such as Kitaev exchange and, directly connected to this, the unconventional magnetic properties of iridium oxide compounds are addressed by wavefunction-based quantum chemical methods and subsequent exact-diagonalization computations for the related effective spin model(s).

Electronic and magnetic properties of defected graphene nanoribbons adsorbed on a single sheet of graphene

Guoda Liepuoniute

From all the research that has been collected since the discovery of graphene, no doubt, it is the material of the future. Excellent electrical and thermal conductivity, elasticity and strong covalent bonds between neighbouring C atoms would make graphene a perfect candidate in semiconductor electronics; however, for this application an energy band gap must be opened. In this work we focus on controlling the size of a band gap while creating defects on zigzag graphene nanoribbons adsorbed on a single graphene sheet. Hydrogenated zigzag ribbons are created of different widths, adsorbed on a sheet of graphene at different distances from each other and doped with nitrogen at varying concentrations. Energy variations and spin properties are tested in order to build a quantum model and present how the energy fluctuates depending on those variables. To achieve this we performed the first-principle calculations using Density Functional Theory (DFT) in the CRYSTAL17 package. Our goal is to create a tunable band gap while simply changing the parameters listed above. We hypothesize that combining semiconducting and magnetic properties in one system, we could construct a device that could be used in quantum information processing, solar cells, spintronic devices or field effect transistors.

A DFT study of copper oxides as photovoltaic absorbers

Aleksandar Živković

The expanding solar technology market has raised interest in exploring p-type semiconductors like copper oxides. Consequently, there is a need for acquiring knowledge about the electronic and optical properties of such materials in order to assess their absorbing potential and solar power conversion efficiency. However, most photovoltaic absorbers are identified using the standard Shockley-Queisser (SQ) selection principle which relies entirely on optimal band gap values. This has been proven as an insufficient criterion as many materials with appropriate values perform badly. We have employed calculations based on the density functional theory (DFT) to assess three copper oxides as potential photovoltaic materials: Cu2O, Cu4O3, and CuO. We created a unique model that describes all three copper oxides accurately. Furthermore, we have assessed their mechanical, electronical, magnetic, and optical properties and linked them to theoretical values of photovoltaic efficiencies. On top of that, we extended the standard SQ limit and answered why copper oxides miss to achieve high solar-absorbing photovoltaic efficiencies despite the fact that they have promising energy band gaps values.

High Temperature Metal-Phthalocyanine Magnetic Molecular Semiconductor

Xuewei Zhang

Organic molecular semiconductors have become very promising candidates for transistors, resistors and photoswitches because of their flexibility, tunable characteristics and ease of manipulation. However, the low magnetic transition temperature makes the operation at room temperature difficult to achieve. Metal-Phthalocyanine (MPc) which possesses a spin-bearing transition metal ion accommodated in the centre of the conjugated ring has been studied extensively due to its combination of semiconducting and magnetic properties. By increasing the strength of magnetic coupling and exchange interaction as well as choosing a suitable central metal, the magnetic transition temperature has the potential to reach room temperature. This research aims to obtain high-temperature MPc-based magnetic semiconductors with novel strategies manipulating the thin film structure. The ideal ferromagnetic system should possess facially stacking structures, strong magnetic couplings, high exchange interactions and magnetic ordering temperatures above the boiling point of liquid nitrogen. Computational simulations by density functional theory combined with D3 dispersion correction and experimental characterisations will be compared. The success of this research will provide a solid foundation for future strategies in obtaining room temperature magnetic molecular semiconductors which could have unprecedented applications in spintronics.

Structural effect of graphitic nitrogen doping in graphene

Liam Harnett

Density Functional Theory simulations using the PBEsol functional and 6-21G* Pople basis set were performed on nitrogen doped graphene supercells. Analysis of the topology of 12x12 sized supercells suggested that the nitrogen atom conformed to the local sp2 hybridisation of the graphene sheet and did not alter the overall topology unless a compressive strain of 2% was applied. The calculated defect formation energies were reasonable for small supercells but deviated significantly from the norm beyond those of 6x6 in size. The results of this investigation may be of interest to those who wish to exploit or mitigate the structural effects of nitrogen-doping in graphene systems.

Strain engineering of phonon thermal transport properties in monolayer 2H-MoTe2

Aamir Shafique

Strain is a very useful and effective tool to enhance the performance of the semiconducting devices. It can tune electronic, optical, and thermoelectric properties. However, the effect of tensile strain on the phonon thermal transport of two-dimensional materials is unpredictable because the flexural acoustic (ZA) mode becomes harder and transverse acoustic (TA) and longitudinal acoustic (LA) modes become softened. The effect of strain on the phonon properties (such as phonon group velocity, phonon anharmonicity and phonon lifetime) and lattice thermal conductivity of the 2H-MoTe2 monolayer is studied by solving Boltzmann transport equation based on first principles calculations. We compare phonon properties and lattice thermal conductivity of the unstrained 2H-MoTe2 to those of the biaxially strained ones. One of the common features of the two dimensional materials is quadratic nature of the ZA mode that disappears by applying tensile strain. We find that lattice thermal conductivity of the monolayer 2H-MoTe2 is so sensitive to tensile strain that it is reduced up to three times by applying 8% biaxial tensile strain due to the reduction in phonon group velocities and phonon lifetime. We analyzed how contribution of each mode in lattice thermal conductivity changes with tensile strain. These results highlight that tensile strain is one of key parameters in engineering phonon transport properties in monolayer 2H-MoTe2 .

DFT INVESTIGATIONS OF 3D C60 POLYMERS WITH ORDERED BINARY-ALLOY TYPE STRUCTURES

Jorge Laranjeira

Three-dimensional (3D) C60 polymerized structures with each molecule adopting one of the two standard orientations, have been studied via density functional theory methods (DFT). The structures investigated were constructed using, as prototypes, well-known ordered binary-alloy (AB) structures - AuCuI,Au3Cu, CuPt, “A2B2” - , in which one standard orientation corresponds to atom A and the other orientation corresponds to atom B. We show that in all the studied structures 56/56 2+2 cycloaddition polymeric bonds are formed between differently oriented molecules but not between similarly oriented molecules. It, thus, corresponds to an orientational antiferromagnetic interaction and the system can be mapped onto Ising fcc antiferromagnet. The bonding type, 56/56 2+2 cycloaddition, is different from the 66/66 2+2 cycloaddition characteristic of the low-dimensional, 1D and 2D, C60 polymers, as it is formed by linking single bonds of neighboring C60 molecules, in contrast what found for the other polymorphs.

These 3D polymer structures are candidates to be obtained experimentally at high pressure once the observed frustration could be relieved [1]. Their structural, elastic and electronic properties were calculated at room pressure and at 9.5 GPa and all were found to be metallic [2].

[1] J. Laranjeira, L. Marques, M. Mezouar, M. Melle-Franco, K. Strutyński, Phys. Stat. Sol.RRL 11 (2017) 1700343.

[2] J. Laranjeira, L. Marques, N. Fortunato, M. Melle-Franco, K. Strutyński, M. Barroso (submitted).

First-principles investigation of the adsorption of carbon dioxide, carbon mono-oxide and oxygen on $CsPbX_3$ (X= Cl, Br, I) surfaces.

Arpit MISHRA, EDF-IPVF

Philippe BARANEK, EDF-IPVF

Andrei POSTNIKOV, University of Lorraine

Abstract

With their ability to be produced at low-cost and high efficiency (22.7%, for MAPI), organic-inorganic halide perovskites may offer a promising alternative to current Si-based technologies. However, the poor stability in the presence of moisture, oxygen, carbon mono-oxide and carbon dioxide stays a major challenge for their commercial applications. In this work, we focus on inorganic halide perovskites i.e. $CsPbX_3$ (X= Cl, Br, I). The adsorption of CO_2, CO and O_2 with the (100) surface of $CsPbX_3$ (X= Cl, Br, I) has been simulated from first-principles using hybrid functionals. Different orientations of CO_2, CO and O_2 have been explored. The results were interpreted in terms of Mulliken population analysis, density of states, vibration spectra and adsorption energy determination. So far, the physisorption of different molecules on the $CsPbX_3$ (X= Cl, Br, I) surfaces were confirmed.

Novel co-crystals based on (benzylthio)acetic acid and selected N-heterocyclic co-ligands

Justyna Sienkiewicz-Gromiuk

Department of General and Coordination Chemistry, Faculty of Chemistry, Maria Curie-Sklodowska University, M. Curie-Sklodowska Sq. 2, 20-031 Lublin, Poland, e-mail: j.sienkiewicz-gromiuk@poczta.umcs.lublin.pl

Co-crystal synthesis has become a field of high interest in the last decade. This category of solid forms has a variety of applications in industries such as molecular recognition and aggregation, molecular biology, pharmacy and nanotechnology [1]. According to the definition, co-crystals are crystalline single phase solids composed of two or more different molecular and/or ionic compounds generally in a stoichiometric ratio which are neither solvates nor simple salts [2].

The study concerns the synthesis, structural and some physico-chemical properties of two novel co-crystals formed between (benzylthio)acetic acid and 2-amino-4,6-dimethylpyrimidine (**1**) or 4,4'-bipyridine (**2**). Co-crystals involving the (benzylthio)acetic and the corresponding N-heterocyclic base synthons were synthesized on the basis of co-crystallization by slow evaporation from a methanol solutions that contains stoichiometric amounts of the components. The resulting co-crystals have been characterized experimentally by SC and powder X-ray diffraction, various spectroscopic techniques (infrared, Raman, ^{1}H and ^{13}C NMR) and thermogravimetric analysis as well as by using DFT theoretical calculations. Crystal structures of analyzed co-crystals reveal that the interactions between the acidic (benzylthio)acetic motif and the basic N-heterocyclic systems occur via strong O−H···N and N−H···O hydrogen bonds.

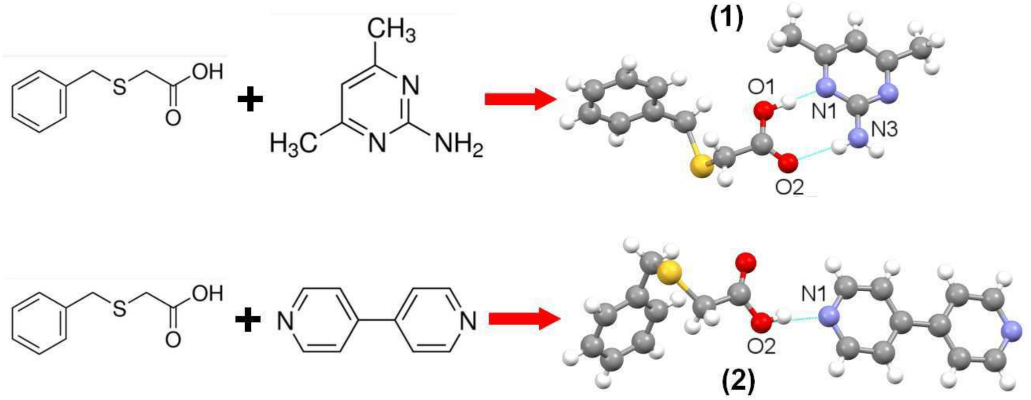


Fig.1. Molecular structure of two components in co-crystals **1** and **2** linked via strong O−H···N and N−H···O hydrogen bonds.

References:

[1] M. Rekdal, A. Pai, R. Choudhari, M.B. Sathyanarayana, *Sys. Rev. Pharm.* (2018) **9**:55-57.

[2] S. Aitipamula, R. Banerjee, A.K. Bansal, K. Biradha, M.L. Cheney, A.R. Choudhury, G.R. Desiraju, A.G. Dikundwar, R. Dubey, N. Duggirala, P.P. Ghogale, S. Ghosh, P.K. Goswami, N.R. Goud, R.R.K.R. Jetti, P. Karpinski, P. Kaushik, D. Kumar, V. Kumar, B. Moulton, A. Mukherjee, G. Mukherjee, A.S. Myerson, V. Puri, A. Ramanan, T. Rajamannar, C.M. Reddy, N. Rodriguez-Hornedo, R.D. Rogers, T.N.G. Row, P. Sanphui, N. Shan, G. Shete, A. Singh, C.C. Sun, J.A. Swift, R. Thaimattam, T.S. Thakur, R.K. Thaper, S.P. Thomas, S. Tothadi, V.R. Vangala, N. Variankaval, P. Vishweshwar, D.R. Weyna, M.J. Zaworotko, *Cryst. Growth Des.* (2012) **12**:2147-2152.

Monoclinic VO_2 nanowire for optical gas sensor application

Prabal Dev Bhuyan[1,4], Sanjeev K. Gupta[1], Ashok Kumar[2], Yogesh Sonvane[3] and P. N. Gajjar[4]

[1]Computational Materials and Nanoscience Group, Department of Physics and Electronics,
St. Xavier's College, Ahmedabad 380009, India

[2]Centre for Physical Sciences, School of Basic and Applied Sciences, Central University of
Punjab, Bathinda, Punjab 151001, India.

[3]Department of Applied Physics, S.V. National Institute of Technology, Surat 395007, India

[4]Department of Physics, Gujarat University, Ahmedabad 380009, India

Abstract

The rising environmental concerns and the effect of pollution on health call; the study of materials for gas sensing achieves rapid speed. However, the development of gas sensors for the detection of toxic gas, calculation of gas concentration in the environment, breath analyzing etc. is paving a way to move forward. Here, we have discussed monoclinic VO_2 nanowire as an optical gas sensor. The monoclinic phase shows semiconducting behaviour with a band gap of 1.17eV. We have adsorbed CO_2, N_2 and SO_2 gas molecules on monoclinic VO_2(M) nanowire to study the interaction behaviour. We have analyzed adsorption energy and relaxation time for the gas adsorbed nanowire. The study of its absorption and transmission properties shows that VO_2 nanowire is likely to open up its application as an optical gas sensor.

Elucidating the Nature of Molecular Rotations on Single-Crystal Surfaces

Kyle Groden[a], Amanda M. Larson[b], Ryan T. Hannagan[b], E. Charles H. Sykes[b,*], Jean-Sabin McEwen[a,*]

[a]The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA 99164

[b]Department of Chemistry, Tufts University, Medford, MA 02155

Molecular machines are a well-known pipe dream in the area of nanotechnology due to their near science-fiction like applications in fields like medicine and materials design.[1] But to bring this dream into reality, we must establish a fundamental understanding of the pieces that would go into building such a device. Molecular rotors have the potential to provide mechanical work for these microscopic devices but originally lacked any element of speed control, which would be essential for any mechanical operation. Although recent studies have shown how chemical environments can influence the speed of these rotors [2], a better understanding of the exact nature of these rotations is desired. In this work, we have used model systems to examine molecular rotations at an atomistic level using *ab initio* calculations. We have found that traditional optimizations were not succifient for modeling molecular rotors and have proposed an alternative scheme for modeling these systems. This scheme was then used to generate accurate rotational potential energies surfaces, from which scanning tunneling microscopy images were generated that agreed well with experimental results. This agreement allowed us to use our potential energy surfaces to examine the possibility of rotational tunneling in these systems. These tunneling studies have shown that quantum tunnelling effects for molecular rotors likely cannot be completely ruled out for any arbitrary system and have also eludicated the effects of barrier shape and height on the quantum tunneling probability.

References

(1) Whitesides, G. M. *Scientific American* **2001**, *285*, 78–83.

(2) Wu, Y.; Wang, G.; Li, Q.; Xiang, J.; Jiang, H.; Wang, Y. *Nature Communications* **2018**, *9*, 1953.

Influences of vacancy and doping on electronic and magnetic properties of monolayer SnS

Hamid Ullah, Mohammad Noor-A-Alam, Hye Jung Kim, and Young-Han Shin*
Department of Physics, University of Ulsan, Ulsan 44610, South Korea

Based on the first-principles calculations, we investigate the structural, electronic, and magnetic properties of defects in monolayer SnS. We study the formation and migration of vacancies at both Sn- and S-sites. In comparison to the S-site vacancy, our calculations show that creating a vacancy at the Sn-site requires lesser energy, indicating that the vacancy at the Sn-site is more likely to be formed in experiments with energetic particle irradiation. For the Sn-rich (S-rich) environment, the vacancy at the S-site (Sn-site) is more likely to be found than the vacancy at the Sn-site (S-site). Reducing the formation of vacancy clusters, the S vacancy remains at the position where it is created because of the high vacancy migration barrier. Both types of vacancies remain nonmagnetic. To induce magnetism in monolayer SnS, we also study the transition metal (TM= Mn, Fe, and Co) doping at the Sn-site and find a significant influence on the electronic and magnetic properties of monolayer SnS. The doping of TM changes non-magnetic monolayer SnS to magnetic one and keeps it semiconducting. Additionally, long-range ferromagnetic behavior is observed for all the doped system. Hence, doping TM atoms in monolayer SnS could be promising to realize a two-dimensional diluted magnetic semiconductor. More interestingly, all the doped TM configurations show a high spin state, which can be used in nanoscale spintronic applications such as spin-filtering devices [1,2].

[1] L. C. Gomes and A. Carvalho, Phys. Rev. B 92, 085406 (2015).
[2] O. V. Yazyev and L. Helm, Phys. Rev. B 75, 125408 (2007).

Reaction Mechanisms for Material Systems with Complex Potential Energy Surfaces

A.-M. Tsopelakou[1], R.P. Lindstedt[1], K. Gkagkas[2]

[1]Department of Mechanical Engineering, Imperial College London, SW7 2AZ, London, UK

[2]Toyota Motor Europe NV/SA, Technical Center, Hoge Wei 33B, B-1930 Zaventem, Belgium

The chemical interactions between surfaces and adjoining fluid phases are often poorly understood and detailed chemistry modeling across scales, starting from the fluid-material surface boundary, is arguably essential for explaining the resulting events. Our aim is to shed light on the development of advanced computational tools that ultimately enable the quantification of interactions between chemical species resulting from advanced engine operation modes and selected metal surfaces (Pt, Rh). The rate parameters for the surface chemistry were derived using a systematic application of Variational Transition State Theory (VTST), for adsorption reactions coupled with two dimensional (2D) collision theory for reactions occurring on the surface. The VTST approach removes the need for the experimental determination of surface sticking coefficients and the associated major uncertainties. The barrier heights were determined using the Unity Bond Index-Quadratic Exponential Potential (UBI-QEP) method. Finally, a thorough analysis of the performance of the detailed chemical mechanisms developed by Kraus and Lindstedt [1,2] and Vincent et al. [3] has been conducted, under fuel-rich conditions over a platinum coated surface in presence and absence of CO co-feed. The reactions of CO over Pt are well-known to be controversial and the current conditions have not been previously studied.

[1] P. Kraus and R. P. Lindstedt, "Variational transition state theory-based surface chemistry for the C_2H_6 /H_2 /O_2 /Pt system," *Energy & Fuels*, vol. 31, no. 3, pp. 2217–2227, 2017.

[2] P. Kraus and R. P. Lindstedt, "Microkinetic mechanisms for partial oxidation of methane over platinum and rhodium," *The Journal of Physical Chemistry C*, vol. 121, no. 17, pp. 9442–9453, 2017.

[3] R. S. Vincent, R. P. Lindstedt, N. A. Malik, I. A. Reid, and B. E. Messenger, "The chemistry of ethane dehydrogenation over a supported platinum catalyst," *Journal of Catalysis*, vol. 260, no. 1, pp. 37 – 64, 2008.

Some Feedback

Overall the feedback was very positive and attendees were very enthusiastic.
Some positive comments have been reported below.

1) Well structured and really help to understand a lot of the nuances of the code. All lecturers were friendly and helpful.

Availability of the lecture/workshop materials outside of the summer school was much appreciated. This will be useful in future revision.

2) Overall, it was the most insightful workshop I have been so far. The lectures were of the highest quality, and it spanned a great range of topics – from fundamentals to some advanced topics. I also appreciated the amount of mathematics/equations in QM discussed. It allows me to understand the CRYSTAL code a lot better. The tutorials were extremely useful. It was great to have all my questions answered and learn how to prepare input file, read them and compute interesting properties. The poster session was great as well. It was fantastic to see how CRYSTAL is used in so many chemistry research areas.

Thanks so much for organising it!

3) The motif of the lectures is to know how CRYSTAL works for different materials applications and it has been fulfilled up to some extend. Tutorials sessions have been the best part of the workshop. I have really enjoyed it a lot.

4) Very nice hand-ons seminars.

5) In the morning sessions all the instructors did their job very well. Overall the morning session was good. The afternoon session was very interesting. Overall the the workshop was very interesting.

6) Lectures very well prepared and speakers for the most part were very good. Very valuable, excellent to have someone helping you to interpret the output! Very clear as well.
Excellent school, very valuable theoretical + practical code usage knowledge.

Would highly recommend to anyone!

7) Transport properties and thermoelectric properties lectures were really helpful. Tutorial were enjoyable. Best part is to go through every basic physics behind the software command.

8) Excellent schedule, organisation and speakers! Very well structured tutorials with lots of practical examples and tips for professionals!

9) I really enjoyed the lectures where you could hear and see the enthusiasm.
Poster session was well organised and excellent opportunity to meet other people and to talk to them in more depth. The dinner was also a good social activity.