



LONDON CENTRE FOR THEORY  
AND SIMULATION OF MATERIALS



## Thomas Young Centre Student Day 2019

Friday 15<sup>th</sup> February 2019  
09.30 to 17.00

Room 120/121 Sir Alexander Fleming building  
Imperial College London

Time	
09:30	<b>Welcome with Tea &amp; Coffee</b>
09.55	Introduction to the TYC Student Day
10.00	<b>Plenary - Energy landscapes: from molecules and nanodevices to machine learning</b> <i>Professor David Wales, University of Cambridge</i>
10.50	<b>Plenary - Dr Jess Wade, Imperial College London</b>
11.30	<b>Tea &amp; Coffee Break</b>
	<b>Student talks</b>
11.45	A configurational energy criterion using discrete dislocation plasticity for the prediction of fatigue crack nucleation sites in Ni superalloys <i>Nikoletta Prastiti, Imperial College London</i>
12.00	Simulation of graphene: exfoliation and superlubricity <i>Robert Sinclair, University College London</i>
12.15	Disordered protein-graphene oxide co-assembly and supramolecular biofabrication of functional fluidic devices <i>Yuanhao Wu, Queen Mary University of London</i>
12.30	Molecular simulation of the adsorption and desorption in angular pores <i>Harry Cardenas, Imperial College London</i>
12.45	<b>Lunch and Posters</b>
14.15	Hot carrier generation from single plasmons in metallic nanoparticles <i>Lara Roman Castellanos, Imperial College London</i>
14.30	Distortions and defects in hybrid halide perovskites <i>Lucy Whalley, Imperial College London</i>
14.45	Ultrafast light-driven electron transfer in a Ru(II)tris(bipyridine)-labelled multiheme cytochrome <i>Xiuyun Jiang, University College London</i>
15.00	Computational methods for photochemistry in molecular crystals <i>Miguel Rivera, Queen Mary University of London</i>
15.15	Defining an optimal metric for the path collective variables <i>Ladislav Hovan, University College London</i>
15.30	On the interplay between conformational complexity, solution structure, and polymorphism in succinic acid nucleation from solution <i>Ilaria Gimondi, University College London</i>
15.45	Thermomolecular orientation and thermodiffusion of asymmetric nanoparticles <i>Juan Olarte-Plata, Imperial College London</i>
16.00	MFF: a python package for automatic force field construction through machine learning <i>Claudio Zeni, King's College London</i>
16.15	Short Break
16.30	<b>Talk and Poster Prize Announcement and Reception</b>

# Plenary Presentations

## **Energy landscapes: from molecules and nanodevices to machine learning**

**Professor David Wales**

**University of Cambridge**

The potential energy landscape provides a conceptual and computational framework for investigating structure, dynamics and thermodynamics in atomic and molecular science. This talk will summarise new approaches for global optimisation, quantum dynamics, the thermodynamic properties of systems exhibiting broken ergodicity, and rare event dynamics. Applications will be presented that range from prediction and analysis of high-resolution spectra, to coarse-grained models and design principles for self-assembly of mesoscopic structures, with recent results for machine learning landscapes.

### **Selected Publications:**

1. Perspective: Energy Landscapes for Machine Learning, PCCP, 19, 12585-12603, 2017.
2. Exploring Biomolecular Energy Landscapes<sup>1</sup>
3. Feature Article: Exploring Biomolecular Energy Landscapes, Chem. Commun., in press, DOI:10.1039/c7cc02413d
4. Perspective: Insight Into Reaction Coordinates and Dynamics From the Potential Energy Landscape, JCP, 142, 130901, 2015.
5. Energy Landscapes: Some New Horizons, Curr. Op. Struct. Biol., 20, 3-10, 2010.
6. Energy Landscapes, Cambridge University Press, Cambridge, 2003

**Dr Jessica Wade**

**Department of Physics**

**Imperial College London**

Physicist and early career researcher in the Department of Physics at Imperial will also give a talk. Her research investigates polymer-based light emitting diodes (LEDs). She also carries out public engagement work in science, technology, engineering, and mathematics (STEM), particularly in the promotion of physics to girls. Jess won the Institute of Materials, Minerals and Mining (IOM3) Robin Perrin Award for Materials Science in 2017, the Institute of Physics (IOP) Daphne Jackson Medal and Prize in 2018 and was included in Nature's 10 people who mattered in science in 2018.

# Poster Presentations

## **Trans-cis proline switches in a pentameric ligand-gated ion channel: How they are affected by and how they affect the biomolecular environment**

Alessandro Crnjar  
King's College London

The 5-HT<sub>3</sub> receptor is a pentameric serotonin-gated ion channel, embedded in the cell membrane of neurons, and is involved in fast synaptic transmission. Its malfunction leads to diseases such as Alzheimer, schizophrenia, drug abuse, and many others. It is also the target of nausea-suppressant drugs. Working on a model of this receptor based on a recent x-ray structure, we investigate a potential trans-cis molecular switch for opening the ion channel, consisting of a proline at the interface between the extra-cellular and the transmembrane domain, as suggested by electrophysiology mutagenesis experiments.

Our study is based on molecular dynamics and free energy calculations with the enhanced sampling method metadynamics, and aims at elucidating, on one hand, the influence of the isomerisation on the gating mechanism, and, on the other hand, the effects of the receptor environment on the isomerisation process.

Our results prove that the isomerisation constitutes a significant step towards the opening of the channel, provoking an important modification at the level of the selectivity filter found at the interface between extracellular and transmembrane domain that may result in an enhanced attraction of sodium ions towards the entrance of the pore.

Our results also highlights how the isomerisation process is influenced by the presence of other protein residues. This not only seems to create preferential paths for the occurrence of this process, but also suggests the possible involvement of some amino-acids in the transmission of the mechanical signal, triggered by the binding of a ligand, down to the transmembrane domain.

## **Estimation of sticking coefficients using mobile and immobile transition states for catalytic platinum systems**

Aliki Marina Tsopelakou  
Imperial College London

The estimation of pre-exponential rate constant factors suitable for microkinetic analysis of reaction pathways in heterogeneous systems requires sticking coefficients. These can either be derived experimentally or, at major computational expense, using ab initio quantum mechanical methods. Even though estimates are available for well-studied systems [1, 2], this is not generally the case, and even for such cases large uncertainties prevail due to incomplete data. The current research uses a theoretical framework for estimating Arrhenius parameters for surface reactions, leveraging the Unity Bond Index-Quadratic Exponential Potential (UBI-QEP) [3] method for estimating barrier heights and the Variational Transition State Theory (VTST) in order to derive surface sticking coefficients for adsorption processes. The present work derives mobile and immobile sticking coefficients and reaction rates for a wide range of temperatures for 31 adsorption reactions and, where possible, compares with experimental data. The potential energy surfaces are explored using the M06 family of density functionals along with either the Stuttgart-Dresden (SDD) or the Los Alamos National Laboratory 2-double-z (LANL2DZ) effective core potentials. The impact of the determined sticking coefficients and reaction rates are compared with previously published reaction mechanisms [2, 4, 5] as well as with related experimental data for platinum catalysts supported on alumina. The ability of the developed method to reproduce the experimental data is explored and the accuracy is compared to the collision theory approach for both mobile and immobile transition states.

1. D. K. Zerkle, M. D. Allendorf, M. Wolf, and O. Deutschmann, "Understanding homogeneous and heterogeneous contributions to the platinum-catalyzed partial oxidation of ethane in a short-contact-time reactor," *Journal of Catalysis*, vol. 196, no. 1, pp. 18 – 39, 2000.
2. R. S. Vincent, R. P. Lindstedt, N. A. Malik, I. A. B. Reid, and B. E. Messenger, "The chemistry of ethane dehydrogenation over a supported platinum catalyst," *Journal of Catalysis*, vol. 260, pp. 37–64, 2008.
3. E. Shustorovich and H. Sellers, "The UBI-QEP method: A practical theoretical approach to understanding chemistry on transition metal surfaces," *Surface Science Reports*, vol. 31, no. 1, pp. 1 – 119, 1998.
4. P. Kraus and R. P. Lindstedt, "Variational transition state theory-based surface chemistry for the C<sub>2</sub>H<sub>6</sub>/H<sub>2</sub>/O<sub>2</sub>/Pt system," *Energy & Fuels*, vol. 31, no. 3, pp. 2217–2227, 2017.
5. 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.

## Polar Domain Walls in Halide Perovskites

Andrew Warwick  
Imperial College London

The perovskite methyl ammonium lead iodide (MAPbI<sub>3</sub>) has recently attracted significant interest<sup>1</sup> in the photovoltaic community owing to its promising power conversion efficiencies, rapidly growing upwards of 23.7%<sup>2</sup>, surpassing that of some existing silicon-based devices. Despite this interest, there are still some open questions regarding the physical properties of MAPbI<sub>3</sub>, such as the role of domain walls which appear in abundance<sup>3</sup>. Domain walls are planar interfaces separating two domains; importantly, emergent functionalities can appear at the interface itself due to the change of structure.

Here, we present density functional theory simulations of domain walls in the inorganic analogue caesium lead iodide, CsPbI<sub>3</sub>, which serves as a starting point towards simulating the more structurally complex MAPbI<sub>3</sub>. We find that tetragonal twins in CsPbI<sub>3</sub> are strongly polar, very thin and, in agreement with their experimental observation, likely to have low formation energies<sup>3</sup>. The emergent polarity at these walls could be part of the origin of MAPbI<sub>3</sub>'s high power conversion efficiency and/or be engineered to enhance it.

1. Li W. et al. Nat. Rev. Mater. (2017), 2, 16099
2. National Renewable Energy Laboratory. Best Research-Cell Efficiencies Chart <https://www.nrel.gov/pv/> (2019) Accessed January 11th, 2019
3. Rothmann M. et al. Nat. Commun. (2017), 8, 14547

## Thermodynamic and Mechanical Properties Prediction of the Zr<sub>2</sub>AlC MAX Phase at High Temperatures

Angeliki Poulou  
Imperial College London

MAX phases are materials known for their excellent stability at high temperatures, and their unique combination of metallic and ceramic properties, a fact that has led to a growing interest in them for many industrial applications. Particularly interesting are MAX phases based on Zr, especially Zr<sub>2</sub>AlC, due to their potential for fuel cladding applications in nuclear power production, where typical operating environments require novel materials able to tolerate high temperatures, oxidizing coolants, and rapid neutron fluences. However, for the case of the Zr<sub>2</sub>AlC phase specifically, there is limited experimental research available and the published theoretical research has mostly focused on zero-temperature conditions lacking accurate derivation of properties at high temperature that require the inclusion of different excitation mechanisms to the free energy.

In this study thermodynamic and mechanical properties of Zr<sub>2</sub>AlC have been calculated at finite temperatures using density functional theory to obtain the free energy including the vibrational contribution and electronic excitations. The vibrational free energy has then been evaluated by employing quasi-harmonic approximation. By utilizing the strain and temperature-dependent free energy, mechanical properties such as temperature-dependent elastic constants and thermophysical volume dependent properties such as isobaric heat capacity and thermal expansion coefficient have been derived.

## **First Steps towards Unravelling the Working Mechanisms of a BODIPY-based Molecular Rotor for Sensing Viscosity**

Bethan Cornell  
King's College London

Fluorescent molecular rotors are molecules with a rotatable part whose fluorescence quantum yield and lifetime are functions of the viscosity and polarity of their local environment. These properties can be exploited to obtain real time imaging of processes involving viscosity changes, which may be signatures of specific diseases. Rotors based on BODIPY have long fluorescent lifetimes and, hence, make excellent probes. However, a detailed description of their working mechanisms at the molecular level has not yet been obtained. We attempt to shed light on these mechanisms by focussing, initially in the gas-phase, on a prototypical rotor: BODIPY-C12, which is composed of a BODIPY-dye core with an attached rotatable phenyl ring.

The ground and excited state potential energy surface of BODIPY-C12 in the gas phase were calculated as a function of the rotation of the phenyl ring (with respect to the core), using Density Functional Theory (DFT), Time-Dependent-DFT and the Restricted Open Shell Kohn Sham (ROKS) method. Minimal energy structures in the S0 state correspond to a twisted geometry. However, in the S1 state both flat and twisted geometries correspond to energy minima. Furthermore, molecular dynamics simulations at room temperature show a complex motion of the phenyl ring, coupling rotation with swinging and out-of-plane distortion of the BODIPY-core. Data from our simulations are compared with experimental absorption and emission spectra and provide interesting insights into the properties of the BODIPY-C12 molecular rotor.

## **Computed phase stability and phase transition mechanisms in CaCO<sub>3</sub> at finite temperature and pressure**

David Carrasco de Busturia  
Imperial College London

First-principles calculations on three known CaCO<sub>3</sub> polymorphs (calcite I, II and aragonite) have been performed using GGA and hybrid exchange density functional theory in the all-electron linear combination of atomic orbitals approximation. The variation of the Gibbs free energy with pressure and temperature has been computed in the quasi-harmonic approximation. The theoretical temperature – pressure phase diagram of the calcite I – calcite II phase transition is compared to the available measurements. In addition, the mechanism of several phase transitions between polymorphs are examined. For example, imaginary phonon frequencies in the aragonite phase suggest pathways to three distinct alternative phases that involve symmetry breaking and distortion of the unit cell. Predictions of the structure for these phases will be reported along with their computed Gibbs free energies.

## **Energetic barriers to the diffusion of C8 aromatic molecules in porous organic cages**

Edward Jackson  
Imperial College London

A large proportion of the world's total energy consumption is used for separation processes, so the development of less energy intensive processes for key separations is a highly important environmental and economic challenge. One such separation is the separation of para-xylene from the other xylene isomers and ethylbenzene, which is difficult using conventional methods due to the molecules' chemical similarity but could be conducted using a shape-selective membrane. This project explores whether porous organic cages, including the imine cages CC3 and CC13, could be used to create such a membrane. Amorphous membranes made of these two molecules have already been made experimentally, and the windows of these cages are similar to the kinetic diameters of these molecules, which implies a shape-selective separation may be possible. Metadynamics was used to quantify the free energy barriers to each C8 aromatic molecule, along with benzene and toluene, exiting individual cages, rotating in the cage void, and diffusing through experimental crystal structures. The sizes of these barriers were related to the structures of the guest molecules. In most cases the exit barrier was significantly larger than the rotation barrier, and there was found to be a correlation between kinetic diameter and exit barrier size, with differences between molecules with the same kinetic diameter explained by substituent effects. This indicates the desired separation may be possible. Differences between the two cages were explained by differences in the range of allowed window diameters for each cage, which were evaluated with molecular dynamics. CC13 is more flexible and has windows that can expand to larger sizes, and therefore had smaller energetic barriers to diffusion than CC3.

## **Singular Metasurfaces: bridging length scales with broadband optical nanostructures**

Emanuele Galiffi  
Imperial College London

Mathematical singularities can be an effective analytic way of describing multi-scale physics. In this work we use singular conformal maps to analytically design and characterise subwavelength metallic structures, which are able to harvest incoming electromagnetic radiation over enormous bandwidths by efficiently excite surface waves. Examples of these structures are surfaces with cusps and gratings of smoothly vanishing thickness. By exploiting this phenomenon, which is interestingly linked to the concept of compacted dimensionality in string theories, we designed a dynamically tunable, extremely broadband THz absorber with a single layer of graphene, whose modulated dynamical conductivity periodically approaches the charge neutrality point. Furthermore, this concept can be extended to any polaritonic system which enables fine structuring, such as hexagonal boron nitride within its reststrahlen bands in the mid-infrared. Via the elegant analytical framework of transformation optics, we provide an insightful explanation of these exotic effects, which are underpinned by the multi-scale nature of singular nanostructures.

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2. Galiffi, E., Pendry, J.B. and Huidobro, P.A. "Broadband tunable THz absorption with singular graphene metasurfaces." *ACS nano* 12.2 (2018): 1006-1013.
3. Galiffi, E., Pendry, J.B. and Huidobro P.A. "Singular Graphene Metasurfaces". *EPJ Applied Metamaterials* (Invited Paper). Accepted

## **From DFT to mesoscopic flow simulations: a machine learning potential for boron nitride**

Fabian Thiemann  
University College London

While a lot of research has been dedicated to the properties and applications of graphene and carbon-based nanomaterials [1], culminating in the award of the Nobel prize to Geim and Novoselov in 2010, the amount of research conducted on the inorganic equivalent boron nitride (BN) is far less [2]. This is even more surprising considering the advantages of BN nanofillers in terms of electrical insulation [3], heat resistance [4], chemical stability and ease of manufacture [5]. BN exhibits an excellent sorption performance for a wide range of organic solvents [6] and shows superior water permeation properties [7] which makes it a promising material for membranes for desalination and water purification [8].

Recently, researchers have been able to tune the nanoporosity of BN to practically any desired range [9]. Nevertheless, a better understanding of the physics behind the adsorption and flow processes of fluids confined within BN-based nanostructures is needed, to guarantee optimal performance of the final product. Traditionally, classical molecular dynamics (MD) are employed to calculate the relevant properties, however, there are doubts about whether the potentials used for the solid-fluid interactions can accurately represent the physical behaviour [10].

To this end, we aim to develop a new potential by applying the Gaussian approximation potential (GAP) machine learning (ML) technique. In contrast to semi-empirical force fields, ML-based potentials do not suffer from the limitations inherent to their mathematical form. In order to faithfully represent the electronic potential energy surface, the GAP model is trained using a database of quantum mechanical (DFT) atomic forces and total energies of structures representative of the relevant regions of phase space [11]. Later, this GAP model should be used to perform adsorption and steady-state flow non-equilibrium MD. Eventually, we hope to have linked macroscopic properties, such as permeabilities or diffusivities, obtained by these simulations to the electronic structure level.

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2. R. Kumar and A. Parashar, *Nanoscale* 8, 22–49 (2016).
3. A. Rubio, J. L. Corkill, and M. L. Cohen, *Physical Review B* 49, 5081–5084 (1994).
4. Y. Chen, J. Zou, S. J. Campbell, and G. L. Caer, *Applied Physics Letters* 84, 2430–2432 (2004).
5. A. Pakdel, Y. Bando, and D. Golberg, *Chemical Society Reviews* 43, 934–959 (2014).
6. W. Lei et al., *Nature Communications* 4, 1777 (2013).
7. C. Y. Won and N. R. Aluru, *Journal of the American Chemical Society* 129, 2748–2749 (2007).
8. G. Tocci, L. Joly, and A. Michaelides, *Nano Letters* 14, 6872–6877 (2014).
9. S. Marchesini, C. M. McGilvery, J. Bailey, and C. Petit, *ACS Nano* 11, 10003–10011 (2017).
10. T. Hilder et al., *Micro & Nano Letters* 5, 150 (2010).
11. P. Rowe, G. Csanyi, D. Alfe, and A. Michaelides, *Physical Review B* 97 (2018).

## **First-principles computational approach to calculate magneto-transport coefficients**

Francesco Macheda  
King's College London

We present a first-principles computational approach to calculate magneto-transport coefficients via the exact solution of the linearized Boltzmann transport equation (BTE). We use DFT and DFPT to describe the electronic and vibrational properties of the system, including electron-phonon interactions; carriers' scattering rates entering the BTE are computed using standard perturbation theory. A similar method has been recently used to calculate thermoelectric coefficients for n-doped silicon in absence of magnetic field. We discuss the application of this approach to p-doped Diamond. In particular, we focus on the effect of the magnetic field on the electronic current and on the Seebeck coefficient, including the phonon drag effect, in a range of temperatures and carrier concentrations; our method is valid for any arbitrary strength and orientation of the magnetic field. This approach gives results in good agreement with experimental data and provides a detailed characterization of thermo-magnetic transport properties of diamond, including magneto-resistance, Hall-coefficient and magneto-Seebeck effect. In this perspective, p-doped diamond is a perfect testing case because of the exceptionally high values of its transport coefficients that make diamond appealing for high-temperature electronics. Future developments will involve the application of our new method to metals, where the magneto-transport coefficient are crucially dependent on the shape of the Fermi surface, or to semiconductors such as SiC, where there are still open questions about the Hall mobility, including its temperature dependence and anisotropy.

## **Atomic Structure, Stabilities and Dynamics of Molecular Clusters of Cement**

Fu Song  
Queen Mary University of London

The work involves characterising the microscopic and mesoscopic structure, dynamics and mechanical properties during and after setting of ordinary (Portland) cement OPC, as true understanding of the atomic-level structure and function remains scarce, particularly with respect to observed mechanical properties. Molecular cluster models based on DFT methods have generated encouraging synergies between experiment and computation. These non-periodic cluster models have no geometric restrictions, therefore are truly amorphous and dynamic. The approach has successfully predicted interfacial structure and dynamics of bioactive dental cements. Hence a battery of neutron and coherent-THz techniques are being employed, guided by the theoretical results, to track the changes in structure, dynamics and functional properties over setting time, OPC and other cementitious systems. D<sub>2</sub>O has been popularly used in detecting dynamic properties during cement hydration process in neutron scattering. We aim to find out the difference between the cement gel mixed with H<sub>2</sub>O and D<sub>2</sub>O.

## **Implementation and performance comparison of queuing algorithms for use in Kinetic Monte Carlo simulations**

Giannis Savva  
University College London

Zacros (<http://zacros.org>) is a Graph-Theoretical Kinetic Monte Carlo software application for simulating molecular phenomena on catalytic surfaces. It implements the first-reaction method for listing and randomly choosing a process to be executed. This method is based on the idea that the next event to be executed has to be the most imminent one, namely, the one with the smallest waiting time. The main task is, therefore, reduced to creating a catalogue containing the waiting time of all realizable events, finding their minimum and updating the time values of the involved processes.

For the above operations to be implemented in a computationally efficient way, different data structures are used. At first, the simple algorithm was implemented, based on storing waiting times in a one-dimensional unsorted array (list) and transversing it element by element to find its minimum. Second, a partially sorted Binary Heap data-structure was tested, offering the advantage of finding the minimum element at constant time. Lastly, Pugh's "Skip List" (1990), a linked-list like data-structure was implemented and further extended to provide us with an almost constant time removal operation.

Appropriate benchmarks enabled us to compare the runtime scaling of the above methods as a function of the total lattice sites using simple but representative chemical reaction models. It was found that the "unsorted list" algorithm exhibits the poorest performance since finding the smallest time value is a considerably slow process. "Binary Heap" performs notably better and seems to share the same performance as "Skip List". Furthermore, the "bottlenecks", namely the operations that potentially hinder performance were clearly identified in each algorithm. Finally, improvements are proposed to further reduce their runtime.

## **Ab Initio Calculations of atomically resolved Phosphorous $\delta$ -layers in Silicon**

Jack Poulton  
University College London

Recent advances in experimental methodologies such as low temperature molecular beam epitaxy have resulted in the possibility of creating scalable donor based quantum computing architectures. In such architectures, atomically precise phosphorous monolayer structures (  $\delta$ -layers) in silicon could potentially act as contact regions or in-plane gates. This work has constructed vacuum separated superlattices using the linear scaling density functional theory code CONQUEST1 to determine the electronic structure of these  $\delta$ -layers. In doing so we obtain an ab initio description of the valley splitting caused by these delta layers as well as values for doping potentials. The effects of dopant disorder and the surface proximity of the  $\delta$ -layers on valley splittings are also investigated. The predictions made in this work extend previous studies by explicitly considering surface effects and may prove useful in interpreting experimental spectroscopic data when constructing  $\delta$ -layer based devices.

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## **Development of tight binding model for zirconium**

Jana Sutna  
Imperial College London

Zirconium alloys are extensively used in nuclear fuel cladding due to their neutron transparency favourable corrosive properties. However, during the lifetime of the cladding, the composition and microstructure of the alloys changes as a result of irradiation damage, hydrogen pickup from the surrounding water, oxide growth on the surface and dissolution and re-precipitation of the alloying elements. The methods currently used for simulation of these effects are either too slow to capture the system size required in the case of density functional theory or lack transferability and reliability in the case of classical empirical potentials, in particular when new elements are added. In this project, we have attempted to build a tight binding potential by following the DFTB approach, which would be transferable over a range of structures and allow for an easy addition of new elements. This allows for a creation of a model with minimal reliability on fitting, which should result in greater transferability. A basis set of 5s 4d 5p orbitals was used for Zr and the errors introduced by going from an LCAO DFT model to a two-center tight binding model with the same basis set have been explored. The basis set needed for simulation of close packed metals is quite long-ranged and the resulting many-body interactions are non-negligible. Corrections were introduced in order to take some of these many-body effects into account for all terms included in the model. However, a satisfactory environment-dependent correction for the hopping integrals is still needed. While some properties are correctly predicted, most notably the electronic density of states around equilibrium, the model still exhibits some unphysical properties away from equilibrium and when defects are introduced.

## **Photodynamic Therapy of C8161 Human Melanoma Cells using Ruthenium Compound**

Julia Tan  
Imperial College London

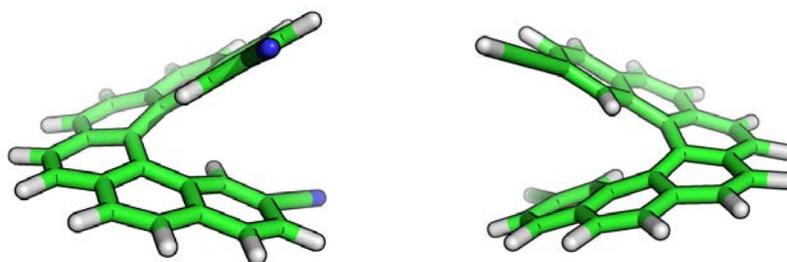
Melanoma is the main cause for skin cancer mortalities. Photodynamic therapy is a promising technique, using oxygen, light and a photosensitising agent to kill tumour cells directly. The photosensitising agent reacts in two different ways to produce highly reactive oxygen species (ROS). Type 1 produces triplet radicals that attack oxygen to form the ROS. Type 2 produces ROS by directly transferring energy to oxygen. Oxygen availability is a limitation of PDT. Thus, anoxic parts is not optimal for PDT to occur. Chemotherapeutic drugs were initially used. However, their undesirable side effects like high toxicity and drug resistance led to the exploration of photosensitising agents. Ruthenium, as a metal, has binding capability to DNA and anticancer properties. Dinuclear ruthenium compounds binds stronger and have more affinity to DNA than mononuclear ruthenium compounds. Ligands, like tpphz, improves localization of photosensitising agents. Because Tpphz-based dinuclear complexes have shown great affinity with quadruplex DNA this experiment will use  $[(\text{phen})_2\text{Ru}(\text{tpphz})\text{Ru}(\text{phen})_2]^{4+}$  to ensure localisation of compound in the tumour cell. This experiment studies the cytotoxicity and phototoxicity of  $[(\text{phen})_2\text{Ru}(\text{tpphz})\text{Ru}(\text{phen})_2]^{4+}$  in concentrations of 0  $\mu\text{M}$ , 10  $\mu\text{M}$  and 100  $\mu\text{M}$ , incubated for 1hour, 16 hours and 24 hours, and are exposed to light dosage with of 1 and 2 hours. Increasing the concentration of the Ruthenium compounds causes a decrease in cell viability. Increasing the incubation period of Ruthenium compounds also decreases cell viability. There is no significant difference when increasing the light dosage from 1hour to 2hours. Hence, as long as there is a high concentration of Ruthenium compound, incubated for 24 hours with 1hour light dosage, there will be significant decrease in cell viability. Future studies include testing at higher concentrations of Ruthenium compound and possibly light dosage of 30 minutes as there might be diminishing effect as the light dosage increases.

## Screening for new chiral organic semiconducting molecular materials using crystal structure prediction

Julia Schmidt  
Imperial College London

Rational design of crystal structures which maximise the material's suitability as an organic semiconductor are undoubtedly of interest to the materials science community. Predicting the spatial arrangement of molecules in the solid state and therefore being able to compute the resulting electronic properties provides valuable structure-property relationships to guide the material design process. Crystal Structure Prediction (CSP) has reported major advances over the last two decades and it is now possible to reliably predict the supramolecular material of large, complex and flexible molecules.<sup>1</sup> Using CSP, we can obtain a set of potential crystal packings for any molecule. We are then able to infer its electronic properties from the packing. The long-standing goal is to use CSP to provide a new avenue for designing organic molecular materials with particular desired electronic properties. This strategy could overthrow conventional trial and error approaches currently employed in the molecule design process.

Recently, we have used CSP to analyse polymorphism in chiral organic molecular materials, and gain insight into the molecular packing effects determining the charge mobility properties of the molecular crystal for [6]helicene and aza[6]helicene.<sup>2,3</sup> Now, we have extended our computational to 2,2-disubstituted helicenes (2,2-dicyano[6]H, 2,2-diethynyl[6]H, Fig.1), which are currently being synthesised by our experimental collaborators in the laboratory.



**Fig. 1** 2,2-disubstituted [6]helicenes: (M)-2,2-dicyano-[6]helicene (left) and (P)-2,2-diethynyl-[6]helicene (right) Helicenes are a class of axially chiral molecules with potential applications as organic semiconducting materials. Previous work on these systems revealed several low-energy helicene crystals with a variety of different molecular packing motifs, we are analysing the most common substructure motifs in the form of one-dimensional (1D) chains. For a given substructure motif, we modify the molecular structure whilst maintaining the packing motif to investigate the impact of terminal substitution on the charge transfer integral.

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## Accelerated sampling of secondary structure formation pathways using digital filtering

Khaled Maksoud

University of Southampton

The dynamics of proteins involve the evolution of slow degrees of freedom (DoF) over timescales that cannot be feasibly simulated within conventional all-atom molecular dynamics (MD) [1,2]. Enhanced sampling methods accelerate the system dynamics such that it can be modelled on a computationally feasible timescale. Many of the commonly used procedures for enhanced sampling, including metadynamics [3] and umbrella sampling [4], involve the modification of the system potential energy by adding bias potential defined with respect to a set of collective variables (CVs) over which the system dynamics are projected.

The selection of appropriate CVs is problematic for many applications of enhanced sampling. Prior knowledge of the system dynamics is required to propose good CVs. Furthermore, any chosen CVs will not directly target the desired degrees of freedom. Digital filtering can be applied in molecular dynamics simulations [5,6] (DFMD, RDFMD) to enhance the velocity components attributed to the targeted DoF. As the targeted DoF is identified by its vibrational frequency range, the only prior information required for filtering is a molecular vibrational spectrum.

Presented here is the implementation of digital filtering to Hamiltonian Monte Carlo simulations – DFHMC. As a principal benchmark, DFHMC, DFMD and RDFMD folding simulations of  $\alpha$ -helix and  $\beta$ -hairpin motifs are tested against secondary structure formation in a range of traditional enhanced sampling simulations.

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## Moving and Vibrating: Study of Magnetic, Electronic and Vibrational properties of Ni<sub>19</sub>

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Based on first-principles all-electron calculations, the structural stability and magnetic variety of Ni<sub>19</sub> nanoparticles has been studied. Exploring the interplay between atomic vibrations and magnetic properties represents an initial and fundamental step in the rational design of nanostructures for application in spintronic and memory devices. Accurate all-electron density functional calculations have been performed on Ni<sub>19</sub> at ab initio level, including several stable isomers and considering perfect and distorted structures. In particular, we report results for bipyramidal (BIP), double- and distorted double-icosahedral (DIH and dDIH), hexagonal close-packed with three layers (3HCP) and four stacked hexagonal close-packed layer (4HCP) nanostructures. These systems have also been studied by adiabatic ab initio molecular dynamics. We found a non-trivial relationship between the relative stability of the nanostructures and the total magnetization for each local minimum, as well as a structure-dependent influence of the total magnetization on the calculated vibrational spectra.

## **Understanding the adsorption mechanism of small organic molecules on Titania surfaces**

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University College London

The application of thin films of organic molecules requires a deep understanding of how molecules interact with both the surface and other molecules. The purpose of this study is to understand the adsorption mechanism of molecules which contain carboxylic acid groups (RCOOH) on TiO<sub>2</sub> surfaces. These molecules are thought to bind to the surface strongly through the RCOOH group, which makes them attractive for their use to develop organic films.

The adsorption of single Coumarin 343 molecules on Rutile TiO<sub>2</sub> (110) surface has been studied using DFT tight binding (TB), which is a semi-empirical method. This method has been chosen to reduce the computational expense that occurs when studying large systems. The first part of this study involved validating that the TB method could produce the geometric and electronic structure of Coumarin 343 and the Rutile TiO<sub>2</sub> (110) surface. The results have shown that both Coumarin 343 and the Rutile TiO<sub>2</sub> (110) surface's geometric and electronic structure calculated by the TB method is in agreement with previous experimental and theoretical data.

The TB method predicts that the adsorption mode where the molecule deprotonates and absorbs in a bidentate fashion is the lowest in energy. The adsorption energy was found to be in -1.90 eV. In this mode the proton binds to a nearby bridging oxygen. This is in agreement with previous experimental and theoretical data. It was found that adsorption energy of this deprotonated model was dependent on the distance of the proton to the molecule.

## **Building CdS and CdSe nano clusters by ab initio random structure search method**

Lei Tan  
Queen Mary University of London

Zero-dimensional colloidal semiconductor nanocrystals are known as quantum dots (QDs), which can be used in biomedical labeling, solar cells, light emitting diodes etc. My research is focused on "magic size" CdSe and CdS quantum dots, that is, these quantum dots contain a well-defined number of atoms and thus a single size, which let the nanoclusters have special properties. However, the atomic structure of these quantum dots are still unknown as experiments data on single crystals from the self-aggregation of the dots is difficult for CdSe and CdS quantum dots.

We have therefore turned to ab initio structure prediction as a useful tool to aid the analysis of experimental observations and develop an understanding of the structures. A systematic first principles structure prediction study of (CdSe)<sub>n</sub> and (CdS)<sub>n</sub> nanoclusters has not been attempted previously, instead guesses are often obtained starting from sections of the bulk crystal that are subsequently relaxed using density-functional theory (DFT). In our research, we have explored the possible space of stable structures of (CdS)<sub>n</sub> and (CdSe)<sub>n</sub> (n up to 34) more completely using ab initio random structure searching (AIRSS)[1,2]. Using AIRSS we build libraries and benchmarks for the ground state structures in a more objective way and also provide some reference to predict the nanoclusters structures with AIRSS method. I will present demonstrate how AIRSS allows us to understand the transition from cage to bulk-like structures.

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## **Modelling the Plasticity of Zirconium Hydrides**

Luca Reali  
Imperial College

The Zr-alloy fuel cladding in fission reactors has to safely withstand thermomechanical cycles in a corrosive environment which causes hydrogen to accumulate ahead of stress raisers leading to hydride formation. Hydrides may break and initiate cracks at whose tip new hydrides form. This is known as delayed hydride cracking (DHC). In addition to this, cyclic plastic strain due to operation conditions leads to the development of slip bands and to a complex network of dislocations, to which completely different failure mechanisms are associated.

The interplay between fatigue and DHC is manifold. Among other things, the dislocations resulting from fatigue are sinks of hydrogen and are likely to interfere with conventional DHC, while at the same time their interactions are altered by the hydrogen Cottrell atmospheres. Moreover, the surface roughening arising from cyclic slip may be the site for DHC nucleation, and the network of hydrides interacts with the fatigue slip bands as well. The model should finally take also radiation damage into consideration, bringing its characteristic population of defects into the picture.

On top of this, the hydrides are hierarchically organised. Macrohydrides spanning the micron to millimetre size are made of stacked platelets of the size of hundreds of nanometres. The effect of atomic diffusion of hydrogen and dislocation slip mechanisms is propagated up to crack nucleating at macroscopic notches. Considering also that the fatigue models have to guarantee a life expectation of several years shows that this problem is inherently multiscale both in space and in time.

## **First Principles Study of the Influence of the Local Steric Environment on the Incorporation and Migration of NO in $\alpha$ -SiO<sub>2</sub>**

Manesh Vinay Mistry  
University College London

Silicon Carbide (SiC) is used as a wide band gap semiconductor which has great potential for high power and frequency application in electrical devices. These applications derive from its many favorable properties like; wide band gap, high thermal conductivity and high breakdown field to name a few. The native oxide of SiC is  $\alpha$ -SiO<sub>2</sub> and is usually deposited onto SiC devices to be used as the gate oxide. The problem with such devices is that there is a high defect density (Dit) near the interface between SiC and  $\alpha$ -SiO<sub>2</sub>. This high defect concentration is remedied by an annealing process usually using Nitric Oxide (NO) as it has been shown to reduce the defect density by 99%.

In this work we give the details of interactions of NO molecules with amorphous ( $\alpha$ )-SiO<sub>2</sub> film and at the SiC/SiO<sub>2</sub> interface are still poorly understood. We use DFT simulations to investigate the NO incorporation energies in  $\alpha$ -SiO<sub>2</sub>, and how these are affected by the steric environment. The results explain the ease with which NO molecules incorporate into  $\alpha$ -SiO<sub>2</sub> and give an insight into the diffusion paths taken during annealing. An exhaustive sampling for exploring NO diffusion pathways uncovered a range of different NO configurations within a completely sampled cell. In the sample, we see a proportional relationship between the degree of steric crowding and the energy of the interstitial.

## **Non-adiabatic processes**

Matt Ellis  
University College London

Non-adiabatic processes play a vital role in many interesting processes such as photosynthesis, respiration and electronic charge transfers. In these systems the Born-Oppenheimer approximation cannot be applied and one must use computational simulations to model the physics. Many techniques have been proposed for this, all of which strike a compromise between accuracy and computation efficiency. To deal with realistic systems that have hundreds to thousands of molecules one must use mixed quantum-classical dynamics where the slow degrees of freedom (the nuclei) are treated classically and the fast ones treated with quantum mechanics. A range of techniques such as the Surface Hopping and Ehrenfest methods have been designed with this in mind. However, they tend to suffer from unphysical over-coherence issues. In this report, I present an implementation of a fragment-orbital based coupled-trajectory mixed quantum-classical algorithm (FOB-CTMQC), which is designed for simulating charge transport in systems of hundreds to thousands organic molecules. This method uses an in-house analytical overlap method (AOM) within the framework of coupled-trajectory mixed quantum-classical (CTMQC) molecular dynamics. CTMQC incorporates decoherence due to two new terms containing a quantity named the Quantum Momentum. I present several numerical tests of my implementation of the method. These include a demonstration of Rabi oscillation, energy conservation and a test of an essential equation used in the derivation of the CTMQC equations. I also discuss a problem in the norm conservation and an implementation of a smoothing function designed to overcome this.

### **Nucleating metastable polymorphs: Novel surface designs found to grow cubic ice under ambient conditions**

Michael Benedict Davies  
University College London

Exploiting desired properties from materials has great importance to many emerging technologies. Changing a materials polymorph is arguably the most fundamental change one can make to its utility. This affects an array of properties ranging from mechanical to the band gap of semiconductors. For instance, polymorphism's effect on physiochemical properties is vital to the pharmaceutical industry. However, obtaining different polymorphs can prove exceptionally difficult when considering metastable states. I will present a methodology for discovering novel surface designs which act as templates for the controlled growth and nucleation of a metastable polymorph.

Taking epitaxy as the inspiration, we first take surfaces cut from the pristine version of the polymorph as a template for growth. Next, we simulate the polymorph's nucleation from the liquid state upon this template. We then extract the contact layer of the polymorph formed on these idealized systems and use this as a structure for further surface designs. Simplifying and refining these extracted surfaces lead to novel designs which nucleate the desired polymorph. We illustrate this method on cubic ice (Ic), the metastable polymorph of Ice I under ambient conditions. A macroscopic crystal of Ic has never been achieved, and it has important possible applications in cryopreservation and weather science. Many different hydroxyl groups designs were discovered to nucleate Ic, and we present interesting novel designs which have no symmetry to the Ic lattice. Our hope is this work will help to achieve this elusive polymorph in experiment and inspire work to achieve other polymorphs in ice and beyond.

### **Super-exchange mechanism and quantum many body excitations in the archetypal hemocyanin di-Cu oxo-bridge**

Mohamed Ali Al-Badri  
Kings College London

We perform first-principles quantum mechanical studies of dioxygen ligand binding to the hemocyanin protein. Electronic correlation effects in the functional site of hemocyanin are investigated using a state-of-the-art approach, treating the localised copper 3d electrons with cluster dynamical mean field theory (DMFT) for the first time. This approach has enabled us to account for dynamical and multi-reference quantum mechanics, capturing valence and spin fluctuations of the 3d electrons. Our approach predicts the stabilisation of a quantum entangled di-Cu singlet in the London-Heitler limit, with localised charge and incoherent scattering processes across the oxo-bridge, that prevent long-lived charge excitations. This suggests that the magnetic structure of hemocyanin is largely influenced by the many-body corrections.

### **A Machine Learning Potential for Carbon**

Patrick Rowe  
University College London

We present recent advances in the development of a machine learning potential for carbon using the Gaussian approximation potential framework. Previous models have demonstrated the accuracy and transferability of GAP models for carbon by focusing on graphene<sup>1</sup> and the amorphous phases<sup>2</sup> respectively. Building on this, we construct a potential which is capable of accurately modelling the properties of both the crystalline allotropes and amorphous phases of carbon, including defects. We demonstrate this transferability by modelling the properties of the crystalline phases, including phonon dispersion curves, formation energies and defect formation energies and structures. Additionally we demonstrate accurate modelling of the liquid phase radial distribution function and the diamond-liquid and graphite-liquid phase coexistence lines of the phase diagram of carbon.

## **Synthesis of N-doped carbon dots film as Interlayer for Enhancing the Photoelectrochemical Performance of Hematite Photoanodes**

Qian Guo

Queen Mary University of London

Hydrogen production by Photoelectrochemical (PEC) water splitting is considered to be a promising strategy to face the forthcoming energy crisis and environmental problems. Hematite ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) with intrinsic key advantages as photoanodes (i.e., it is abundant, environment-friendly, corrosion-resistant, and visible-light active) has been intensively studied in recent years. However, it also suffers from inherent shortages like terrible conductivity, short hole diffusion length (2-4 nm), and poor carrier lifetime ( $\sim$ 10-12 s), which results in its practical maximum efficiency is still far from both the benchmark and theoretical maximum solar-to-hydrogen (STH) efficiencies.

Carbon dots (CDs), as a new member of carbon materials family, have shown some unique properties such as light harvesting, down- and up-converted photoluminescence (PL), and photoinduced electron transfer ability, which can help to broaden the photoabsorption and promote the separation of photogenerated charge carriers when coupled with other semiconductors as photoanodes. Therefore, in this study, N doped carbon dots (NCDs) were synthesized and used to improve the PEC performance of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> photoanodes by serving as an interlayer between  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> nanorods and FTO substrate. The results demonstrated that NCDs film as interlayer between FTO substrate and hematite nanorods exhibits positive effects on the PEC performance of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> photoanodes by promoting photogenerated electron transfer, thus reducing the onset potential of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> photoanodes by 0.1 V vs. RHE and enhancing the photocurrent density by 52% at 1.23 V vs. RHE.

## **Modelling Defect Structures in TCO**

Qing Hou

University College London

We present a consistent interatomic force field for In<sub>2</sub>O<sub>3</sub> and SnO<sub>2</sub> that has been derived to reproduce lattice energies and, consequently, the oxygen vacancy formation energies in the respective binary compounds. The new model predicts the dominance of Frenkel-type disorder in SnO<sub>2</sub> and In<sub>2</sub>O<sub>3</sub>, in good agreement with ab initio defect calculations. The model is extended to include free electron and hole polarons, which compete with charged point defects to maintain charge neutrality in a defective crystal. The stability of electrons and the instability of holes with respect to point defect formation rationalizes the efficacy of n-type doping in tin doped indium oxide (ITO), a widely employed transparent conducting oxide in optoelectronic applications. We investigate the clustering of Sn substitutional and oxygen interstitial sites in ITO, finding that the dopants substitute preferentially on the cation crystallographic d site in the bixbyite unit cell, in agreement with experiment. The force field described here provides a useful avenue for investigation of the defect properties of extended transparent conducting oxide systems, including solid solutions.

## **Stochastic Multireference Perturbation Theory**

Robert Anderson

King college London

Abstract: Multireference perturbation theory improves upon active space electronic structure approaches by including interactions with the external orbital space. Implementations of MRPTs have been based on exact deterministic solvers, which quickly become impractical as the active space is enlarged to encapsulate more static correlation. Here we present an adaptation to the FCIQMC algorithm which realises the stochastic estimation of MRPT2 energies for larger active spaces.

## Surface diffusion and step edge adhesion of Co-Salen on a bulk NaCl (100) surface

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The self-assembly of metal-organic molecule, Co-Salen (Co(C<sub>16</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>)), on a NaCl(100) surface, has been investigated using NFAFM. At room temperature, two different morphologies have been observed; A metastable nanowire and a stable nanocrystallite, both believed to consist of Co-Salen dimers units[1]. However, from low temperature measurements it is known that the Co-Salen is individually deposited and adsorbed onto the surface. Experimentally, dimerization is observed at already decorated step edges. Furthermore, it is observed that step decoration occurs first at the upper terrace of a step, but that the nanowire growth starts from the lower terrace of a decorated step edge. It is unclear from the experimental results what role the step edges have in the formation of molecular dimers.

In this work, we present a Density Functional Theory (DFT) based investigation into surface diffusion and step edge adhesion of Co-Salen molecules at non-polar step edges of the NaCl(100) surface.. On flat terraces it has been shown that the Co-Salen molecule weakly binds to the surface in two main configurations centred on the Cl sites, one along the <110> direction and a second along the <100>, with 0.6 eV and 0.5 eV adsorption energy respectively [2]. Barriers for diffusion have been calculated and shows dependence both on the orientation of the molecule, and the translation direction of the molecule. Translation along the <110> direction when in the global minimum configuration, has been shown to be 0.4 eV or 0.1 eV, due to two inequivalent translation directions. When oriented along the <100> direction, the barrier to translate in the two orthogonal <110> directions, is at average 0.2 eV with a small difference due to the chirality of the molecule.

Upon adsorption at a step edge, the molecule gains 0.2 eV, and is at a site half way between the top and bottom terrace.

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## The effect of magneto-optic coupling on plasmons at the surfaces of topological insulator

Samuel John Palmer  
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Although there has been much interest in the electronic properties of topological insulators—materials with insulating bulks and conducting surface states—relatively little attention has been given to the optical properties of these systems. It was shown recently [1] that the exotic surface states of topological insulators create a magneto-optical coupling effect in the material. Normally this magneto-optical coupling effect is very weak, but we demonstrate a significant enhancement when using typical prism coupling apparatus to excite plasmons at the surface of topological insulators, observed as a polarisation rotation of the plasmon.

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## **Atomistic Non-Adiabatic Molecular Dynamics Simulations of Charge Carrier Transport in Organic Materials.**

Samuele Giannini  
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Exciting new technologies such as organic light emitting diodes, photovoltaics and nanoelectronics rely on organic semiconductors. While important progress has been made in recent years towards theoretical and computational modelling of organic semiconductors (OSs), understanding the charge transport (CT) mechanism in these materials is still very challenging because the parameters determining the dynamics are typically outside the regime of validity of existing theories (e.g. Hopping or Band theories). On the other hand, non-adiabatic molecular dynamics simulations are in principle free of model assumptions permitting an “ab initio” view into the CT mechanism. We have recently developed an efficient decoherence-corrected surface hopping methodology (denoted FOB-SH) which allows us to propagate the coupled electron-nuclear motion in realistic condensed phase systems [1-3]. Here we present the first application of FOB-SH to the calculation of room temperature charge mobility for a series of eight molecular organic crystals. We obtain very good agreement with experimentally measured mobility values over three orders of magnitude successfully bridging the regime where hopping and band models are invalid. We find that the mechanism of transport critically depends on the ratio between electronic coupling ( $V$ ) and reorganization energy (electron-phonon coupling,  $\lambda$ ),  $V/\lambda$ . At small ratios, as found in naphthalene, anthracene and pyrene, the charge carrier is delocalized over no more than 1-3 molecules and diffuses through the crystal via hopping. For values exceeding the critical threshold  $V/\lambda > 1/2$ , as found in pentacene and rubrene, the charge carrier forms a polaron delocalized over 10 or more molecules concomitant with a strong increase in mobility. Implications of our work for the search of new organic materials with high room temperature mobility will be discussed.

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## **The microscopic Einstein-de Haas effect**

Tomos Wells  
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The Einstein-de Haas (EdH) effect, which transfers spin angular momentum to mechanical angular momentum, was established experimentally in 1915. While a semi-classical explanation of the effect exists, modern electronic structure methods have not yet been applied to its understanding. In this poster we investigate the microscopic origins of the phenomenon by means of a non-collinear tight-binding model of an O<sub>2</sub> dimer. By varying an external magnetic field in the presence of spin-orbit coupling, a torque can be generated on the dimer, validating the presence of the EdH effect. Avoided energy level crossings and the rate of change of magnetic field determine the evolution of the spin. Other contributions to the torque exerted on the nuclei arise from field-induced changes in the electronic orbital angular momentum and from the direct action of the Faraday electric field associated with the time-varying magnetic field on the charges in the molecule.

## **Towards the understanding of electronic properties of twisted bilayer graphene**

Zachary Goodwin  
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It has recently, and somewhat unexpectedly, been discovered that twisted bilayer graphene (tBLG) exhibits insulating and superconducting behaviour at certain temperatures. Since the discovery, there has been tremendous interest from theoretical communities to rationalise these observations. We study twist-angle dependent electronic properties of tBLG using a tight binding model that is able to handle the large unit cells associated with the tBLG Moiré lattice. The model accounts for atomic corrugation in the out-of-plane direction, which leads to energy gaps between the flat bands near the Fermi energy and the other bands (in agreement with experiment). We use our model to calculate the dielectric response function of tBLG in the constrained random phase approximation, which enables determination of the screened interaction between electrons in the flat bands. We also calculate the Wannier functions associated with these bands, from which a model Hamiltonian is obtained that can be used in state-of-the-art functional renormalisation group methods to calculate the electronic phase diagram of tBLG. Our approach naturally lends itself to systematic improvements and to application to other bilayer materials.