The Two-Dimensional Materials Symposium
Wednesday 24th March 2021
14.00 – 17.20

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Chairs:
Dr Cecilia Mattevi
Professor Sandrine Heutz

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Abstracts:

**Inkjet printed circuits with two-dimensional semiconductors for high-performance electronics**

Dr Felice Torrisi, ICL

Air-stable semiconducting inks suitable for complementary logic are key to create low-power printed integrated circuits (ICs).[1] High-performance printable electronic inks with two-dimensional (2D) materials have the potential to enable the next generation of high performance, low-cost printed digital electronics.[2] In this talk I will demonstrate air-stable, low voltage (< 5 V) operation of inkjet-printed n-type molybdenum disulfide (MoS2) and p-type indacenodithiophene-co-benzothiadiazole (IDT-BT) field-effect transistors (FETs), achieving a mobility of up to 0.1 cm2V−1s−1 and estimating an average switching time of tMoS2 ~ 4.1μs for the MoS2 FETs.[3] This is achieved by engineering air-stable MoS2 and IDT-BT inks suitable for inkjet-printing complementary pairs of n-type MoS2 and p-type IDT-BT FETs, complementary logic inverters with a voltage gain |Av| ~ 4. Finally, I will discuss the charge transport mechanisms of simple surfactant- and solvent-free inkjet-printed thin-film devices with 2D materials.


**Charged graphene as a versatile precursor for multifunctional grafting**

Dr Noelia Rubio-Carrero, ICL

Graphene has attracted increased attention in recent years due to its exceptional electronic, optical, mechanical and thermal properties. However, the exfoliation of graphite is critical to improve the compatibility of graphene with processing solvents and to introduce electrostatically stabilising and/or tagging moieties. Graphite intercalation compounds (GICs) are well-known precursors that afford isolated graphene layers avoiding framework damage; we have used this method to modify graphene with a variety of small molecules, polymers, metallic nanoparticles or single Pt atoms. Tuning these functionalities allow us to prepare a wide variety of modified graphene systems for different applications. In this presentation I will review different approaches for the preparation of modified graphenes and its use in polymeric composites, fuel cell electrodes and as protein nucleation agents among others.
2D materials for heterostructures and miniaturized microwave biosensors  
Dr Antonio Lombardo, UCL  

Semiconductor-based heterostructures play a major role in modern integrated electronics and optoelectronics. 2D/layered materials (2DLM) offer a new platform for heterostructures, enabling deterministic stacking of crystals with very different properties, incommensurate lattice and arbitrary mutual rotation. I will briefly introduce a process to deterministically stack 2DLM with atomically clean interfaces and achieve very high mobility in graphene field effect transistors. In the second part of the talk, I will present some recent experimental and simulation results on atomically-thin microwave biosensors, were graphene coplanar waveguides are combined with microfluidic channels to identify specific DNA sequences.

Lignin-derived electrospun mats incorporating graphene oxide for Na-ion batteries  
Dr Maria Crespo Ribadeneyra, ICL  

Energy technologies rely on the production of efficient materials and their production normally relies on a huge supply of energy. To keep a balance, we need to minimise the energy we employ to produce these materials, starting from which precursors we chose for their synthesis. In this context, we propose to produce low-cost energy components for non-geopolitically compromised rechargeable Na-ion batteries from sustainable and abundant precursors. Carbon nanofibre mats have been electrospun from a sustainable biomass precursor (Lignin) incorporating low loadings of graphene oxide (GO) as nanocharges. Through the synergistic effect between GO and lignin after thermal treatment, properties such as porosity, graphitic degree, surface area, electrical conductivity and flexural modulus of the mats were tuned. In this short talk we present preliminary data on the influence of the above properties on the performance of the mats as 3D current collectors and electrodes for Na-ion batteries.

Magnetism and spintronics in the flat land - is that exciting?  
Prof. Hidekazu Kurebayashi, UCL  

I would like to introduce some recent development of the research field on magnetic 2D van der Waals materials. It is essentially magnetic graphene where some of ions within a layer of these materials have individual moments and most importantly they are coupled to show a magnetic order. I will show representative material systems within this field and how their magnetic properties can be controlled by external stimuli such as electric field, including work performed by LCN scientists.

Nanophotonic antennas boost the light emission from a MoS2 monolayer  
Dr Riccardo Sapienza, ICL  

I will describe recent experiments with monolayers of WSe2 coupled to GaP dimer antennas which, through a combination of enhancement of the spontaneous emission rate, favourable modification of the photoluminescence directionality and enhanced optical excitation efficiency, can reach an signal enhancement of 3-orders of magnitude [1]. I will conclude with an outlook on different nanoscale approaches to tailoring the local density of optical states (LDOS) in dielectric nanostructures, based on the phase distribution of the scattered optical fields induced by point-like emitters, which can reach Purcell enhancements of over 1000 [2].


Modelling charged defects in two-dimensional materials
Dr Johannes Lischner, ICL

A detailed understanding of defects is needed for applications of two-dimensional (2D) materials in future technologies. Charged defects, in particular, are important because of their diverse roles as donors, acceptors, traps and scattering centers. However, modelling such defects is highly challenging because the weak dielectric screening of 2D materials results in long-ranged defect potentials. In this talk, I will present a novel multi-scale approach to address this problem. In this method, the screened defect potential is obtained from ab initio density-functional theory calculations and then used as input into a large-scale tight-binding calculation. This allows the modelling of systems containing 100,000 atoms or more. I will present results for charged defects in graphene, transition-metal dichalcogenides and also phosphorene and demonstrate that our calculations are in good agreement with scanning tunneling spectroscopy measurements.

Hall scattering factor in graphene from first principles
Dr Nicola Bonini, KCL

Hall measurements of graphene are of fundamental importance to access key physical information like the carrier concentration and the drift mobility of samples. However, the accurate determination of these quantities relies on the knowledge of the Hall scattering factor. In experiments this factor is commonly assumed to be 1, but this assumption is based on studies done on 3-dimensional semiconductors with quasi-parabolic band dispersion. Graphene instead is a two-dimensional material characterised by a linear dispersion of the electronic bands and non-trivial carrier scattering rates. Here we present a first-principles study of this quantity computed via the exact solution of the Boltzmann transport equation for electrons in presence of both an electric and a magnetic field. Our results show that while at high carrier densities, the factor is around 1 in a wide temperature range, at low doping its temperature dependence is very strong with values that are as high as 4 below room temperature and as low as 0.6 above room temperature. This unique behaviour is due to both the electronic structure and the peculiar coupling between electrons and phonons in graphene.