HOWDI : THEMATIC SCHOOL “ADVANCED PHYSICS OF VAN DER WAALS HETEROSTRUCTURES”

ROSCOFF, 24-30 SEPT. 2023

SCIENTIFIC PROGRAM

MAIN LECTURES :

1- INTRODUCTION TO VDW HETEROSTRUCTURES (1H30) : FENG WANG (H, BERKELEY, USA) EMAIL: FENGWANG76@BERKELEY.EDU

Tentative outline:
(1) General introduction of van der Waals heterostructure as synthetic quantum materials.
(2) Using moire superlattice as a generic route for engineering strong correlation: no magic angle is necessary. Using TMD moire superlattice at zero twist angle as examples.
(3) TMDC moire excitons (can skip if it is covered in other talks.)
(4) Microscopic understanding of moire heterostructures: imaging moire reconstruction, flatband, moire potential landscape, generalized Wigner crystals, and other features using STM-based techniques.

2- BOTTOM UP FABRICATION OF VDW STACKS (2X 1H30) : SANG-HOON BAE (H, WASHINGTON UNIV., USA) EMAIL: SBAE22@WUSTL.EDU

Bottom-up fabrication of vdW stacks: direct growth of heterostructures

1. Importance of heterostructures
2. History of 2D materials and van der Waals (vdW) materials
3. Introduction to vdW heterostructures
4. Traditional Fabrication vs. Bottom-up Approach
5. Techniques for bottom-up approach
6. Comparison between 3D material growth and 2D material growth
7. Catalytic growth: Graphene
8. Si sublimation of SiC for epitaxial graphene

9. Catalytic growth: BN
10. Non-catalytic growth through kinetic control for other 2D materials
11. Single crystal growth: epitaxy
12. Single crystal growth: confined growth
13. Freestanding 3D nanomembranes for vdW stacks
14. How to produce 3D nanomembranes
15. 2D materials-assisted layer transfer
16. Artificial heterostructure

3- TOP DOWN FABRICATION (1H30) : **R. GORBACHEV** (H, MANCHESTER, GB) EMAIL: ROMAN@MANCHESTER.AC.UK

Pt1.
1. Introduction: mechanical exfoliation of bulk crystals
2. Basic properties of graphene and importance of its substrate
3. The concept of materials design using layer-by-layer assembly
4. Brief overview of key materials involved
5. Overview of state-of-the-art transfer techniques
6. Contamination types and its characterisation
7. Mitigation strategies for interlayer contamination
8. Novel polymer-free transfer
9. Layer assembly in UHV

Pt2.
10. Structural homogeneity of 2DM in heterostructures
10. Moiré superlattices: atomic structure overview
11. Reconstruction regime in twisted interfaces: atomic structure
12. Homogeneity of moiré lattices: current challenges
13. Basic properties of reconstructed lattices
14. Recent progress in studies of reconstructed domains.

4- ADVANCED STRUCTURAL CHARACTERIZATION OF VDWH : TR-ARPES (2X 1H30) : K. DANI (H, OKINAWA, JP) EMAIL: KMDANI@OIST.JP

Viewing light-induced phenomena through the lens of a Momentum Microscope

In these lectures, I will review the broad techniques associated with ARPES – Angle Resolved Photoemission Spectroscopy; as well as the scientific breakthroughs made possible with this instrumentation, particularly in the context of two-dimensional semiconductors.

In the first part of the lectures, I will survey the instrumentation, and associated developments in the field. Therein, I will briefly review the concept of band-structure characterization using the classical ARPES technique. I will then briefly introduce the ARPES variants: μ-ARPES, spin resolved (SR) ARPES, and time resolved (TR) ARPES, including their unique virtues and constraints. Finally, I will introduce the emerging platform of momentum microscopy and show how it can serve as an efficient tool to perform multi-dimensional photoemission spectroscopy.

In the second part of the lecture, I will discuss the progress in investigating 2D materials with ARPES. In particular, we will focus on a series of recent breakthroughs that have enabled the visualization of few particle composite states, such as excitons, in momentum space, using TR-ARPES based techniques.

5- ELECTRONIC PROPERTIES OF 2D MATERIALS + MOIRÉ PHYSICS (3 X 1H30) : M. GOERBIG (H, ORSAY, FRANCE) EMAIL: MARK-OLIVER.GOERBIG@UNIVERSITE-PARIS-SACLAY.FR

outline:
i. start with the graphene band structure as a prototype for 2D crystals (calculation in the simplified tight binding model, with one pz orbital per site)
ii. emergence of Dirac fermions as a low-energy model in structures with at least two bands
iii. band structure of TMDC (monolayer), role of spin-orbit coupling, relevance of Dirac fermions
iv. geometric and topological aspects in 2D crystals, implications for spectral properties, electrons in 2D crystals under strong magnetic fields
v. opening up to heterostructures, moiré patterns

6- ELECTRONIC PROPERTIES 2 (TIGHT BINDING APPROACHES) : S. LATIL (H, SACLAY, FRANCE) EMAIL: SYLVAIN.LATIL@CEA.FR

Electronic properties: generalities
 * Born-Oppenheimer approximation
 * N-body electronic problem
 * Hartree-Fock
 * DFT in the Kohn Sham picture

- Tight-Binding model(s)
 * simplest (Huckel)
 * translational symmetry in crystals: Bloch theorem
 * examples: h-BN and graphene in their simplest approaches (1st nearest neighbors)
 * more refined TB: /= orbitals per site, Slater-Koster, non-orthogonal basis sets, etc.
 * practical TB: problem of parametrization, portability and reliability
 * example: AB and twisted bilayer graphene

- How to use symmetry with a TB model?
 * rectangular graphene quantum dot (mmm or D_2h group)
 * triangular graphene QD (using the 3 axis rotation)
 [* rotations of d orbitals (needed for TMD)]
 [* last example: graphene antidot lattices and the introduction to the
 concept of 2D supercell]

- Some useful TB treatments and analyses
  * Dipolar transitions in the TB scheme
 [* application of a B field or a V potential]
 [* diagonalization vs. O(N) techniques.]

- Moiré patterns of hexagonal 2D systems
  * rotation with coincidence
  * Moiré homostructures by means of asymmetric supercells
  * example: construction of graphene moiré supercells
  * example: construction of BN (or TMDs) moiré supercells
  * supercells HETEROstructures, why it is more complicated?
  * symmetry: p3, p321, p312 and p622 symmetry groups -> number of nonequivalent atomic sites
  * symmetry: how to use it practically with TB model and moiré structures?

[[- Introduction to excited states
  * general problem (within N-body scheme)
  * excited states in TB]]

7- PHONONS AND ELECTRON-PHONON INTERACTION OF 2D HETEROSTRUCTURES (2 X1H30) : J. MAULTZSCH (F, ERLANGEN, G) EMAIL: JANINA.MAULTZSCH@FAU.DE

- short intro to phonons (why phonons at all) and (resonant) Raman
- intro to general aspects of phonons in layered crystals
- phonons in vdW layers (TMDCs, graphene, hBN) vs. stronger interacting layers (e.g. Sb, bP)
- phonons in vdW heterostructures and in twisted bilayers
- Raman: resonances / double-resonances in graphene and (twisted) bilayer graphene
- electron-phonon coupling: general aspects (how to determine in theory/Raman)
- electron-phonon coupling in TMDCs (if you want also in graphene)
- electron/exciton-phonon interaction in TMDCs related to optical spectra

8- TRANSPORT PROPERTIES AND QUANTUM TRANSPORT IN 2D MAT AND VDW HETEROSTRUCTURES (4X 1H30) : C. **STAMPFER** (H, AACHEN, G) EMAIL: STAMPFER@PHYSIK.RWTH-AACHEN.DE

· Basics of electron transport in 2D, incl. limits of the Drude model and characteristic length scales.

· Electron scattering in graphene, Klein-tunneling, the origin of the ultra-high carrier mobility in graphene and the role of strain

· Quantum point contacts in graphene, high tunability of the Fermi wavelength in graphene and viscous flow. Soft-confinement in gapped BLG and quantized conductance.

· Transport through bilayer graphene quantum dots. Sequential tunneling, bias spectroscopy and perfect electron-hole symmetry. The role of Berry curvature for controlling the valley degree of freedom.

9- OPTICAL PROPERTIES (EXCITONIC PHYSICS INCL. INTERLAYER EXCITONS)(2 X 1H30) : ALEXEY CHERNIKOV (H, Dresden, G) email: alexey.chernikov@tu-dresden.de

Outline:
Lecture 1: Basic properties of excitons in 2D
- Concept of Coulomb-bound electron-hole pairs
- Implications of 2D confinement and dielectric screening
- Selected experimental methods to study excitons (STS, optics & magneto-optics)
- Light-matter coupling & spin-valley selectivity

Lecture 2: Exciton in external fields, mobility & heterostructures
- Exciton-carrier complexes and magneto-optical effects
- Exciton diffusion: influence of disorder and interactions
- Excitons in heterostructures: interlayer, dipolar excitons, Moiré potentials

10- SPINTRONICS - EXPERIMENTAL (1H30) : **MARTA GALBIATI** (F, ESP.)

EMAIL: MARTA.GALBIATI@UV.ES

- Introduction to 2D materials for spintronic devices
- Device fabrication
- Focus on spin valve devices with spin filter and interface effects

11- SPINTRONICS - THEORETICAL (1H30) : **S. ROCHE** (H, ESP.) EMAIL: STEPHAN.ROCHE@ICN2.CAT

Theoretical Spin transport in 2D materials and heterostructures
- Spin dynamics, relaxation mechanisms and the role of intraparticle entanglement
- Proximity effects and spin transport anisotropy
- Enhanced spin-orbit coupling and spin current generation
- Topological spin transport and canted spin transport regimes (SHE and QSHE)
- Spin-orbit torque physics

12- Magnetism in 2D Materials and vdWH - experimental (1h30) : J. Coraux (H, Grenoble, France) -EMAIL: JOHANN.CORAUX@NEEL.CNRS.FR

- Historical perspective
- Target properties
- Materials science considerations: material library, preparation vs growth, stability issues, characterization techniques
- Evidences of magnetism with 2D character
- Demonstration of the manipulation of 2D magnetism
- Spin textures in van der Waals and 2D magnets
- Magnetic van der Waals heterostructures: proximity effets, spin-dependent electronics
- Prospects

13- 2D MAGNETISM - THEORY : **JOSE LADO** (H, AALTO, FINLAND) EMAIL: JOSE.LADO@AALTO.FI

- General introduction to 2d magnets
- Origin of magnetic interactions: exchange and superexchange
- Magnons and the role of magnetic anisotropy
- 2D multiferroics
- 2D spin liquids and spinons
- 2D Kondo magnets

14- TWISTRONICS AND MOIRÉ PHYSICS (1H30) : **R. RIBEIRO** (F, SACLAY, FRANCE) EMAIL: REBECA.RIBEIRO@UNIVERSITE-PARIS-SACLAY.FR

Aligned graphene/BN systems: The main point of the lecture will be to show the effects of the moire starting from a simple system (graphene) to a more complicated one (twisted bilayer graphene). For this I will use the large palette of experimental phenomena that can be observed in these systems.
- Monolayer Graphene/BN: modification of the electronic band structure and topological effects
- Bilayer graphene/BN: ferroelectricity, superconductivity?
- Doubly-aligned monolayer and bilayer graphene: moire composite or quasicrystal behavior
- Twisted bilayer graphene at magic angle: superconductivity and correlations (short version)
- Twisted bilayer aligned with BN: quantum anomalous Hall effect

15- VDW HETEROSTRUCTURES FOR Q TECHNOLOGIES (1H30) : **B. GERARDOT** (H, EDINBURGH, GB) EMAIL: B.D.GERARDOT@HW.AC.UK

2D materials for quantum technologies

1. Introduction to quantum optics and state-of-the-art examples
    1. Single photon sources
    2. Spin-photon interfaces
    3. Cavity / waveguide QED
2. Introduction to quantum technology
    1. Quantum networks and communication
    2. Quantum sensing
    3. Q simulation
3. 2D material landscape
    1. Defects in hBN
    2. Quantum emitters in TMDs
    3. Moire superlattices
4. Challenges / Perspectives / Opportunities for 2D materials

SEMINARS

Carmen Rubio Verdu (ICFO, Spain): carmen.rubio@icfo.es

PRACTICALS

SIMULATIONS : IACOPO.TORRE@ICFO.EU

For the simulation practical sessions, please ensure that you bring your personal laptop.
You need to install before the school the following components:

-Python 3
-jupyter notebooks
-modules : numpy, scipy, matplotlib.
We suggest to install anaconda to get all the previous items.

-the package pybandstructure that can be obtained via
pip install pybandstructure
-the package diffusive-solver that can be otained via
pip install diffusive-solver
-FEniCS version 2019.1.0
See installation instruction at https://fenicsproject.org/download/archive/

EXFOLIATION, TRANSFER AND STACKING : SHIESTAND@PHYS.ETHZ.CH

RAMAN & PL SPECTROSCOPY AND MAPPING : **OPHELIE.LANCRY@HORIBA.COM**