MANO

1st semester - Winter Workshop, 15-16 December 2022
Lecture room n.1 level -1

MAterials Physics and NaNOscience

During the MANO Winter Workshop, two scientists from renowned institutions will be invited to give lectures / seminars, the two invited speakers for this semester are:

Prof Franco Caccialli, *UCL, Dept of Physics and Astronomy* *https://www.ucl.ac.uk/physics-astronomy/people/professor-franco-cacialli*

Dr. Bridget Murphy Kiel Nano, Surface and Interface Science Priv.-Doz. Dr. Bridget Murphy — Kiel Nano, Surface and Interface Science (KiNSIS) (uni-kiel.de)

The detailed timetable of the workshop will be published on the Physics master website.

The students of the MANO curriculum are **warmly encouraged** to prepare a poster on a specific topic, a list of possible topics is proposed below.
The posters will be prepared by groups of **two students**. The students will participate to the competition for the best presentation award.
Besides the proposed topics, the students are free to propose other topics that must be discussed in advance with one of the teachers of the first semester courses. Note that the workshop will be held in presence.
The student activity will be recognized with **3 CFU** within the course: *Advanced Professional and Research Skills in Physical Science* (2^{nd} year, 2^{nd} semester) through the presentation of a certificate of attendance.

Detailed instructions:

1. The workshop will be organized in presence.
2. For poster presentation /printing the students will receive further info.
3. The student groups must be organized in advance, and *the name of the components of the group and the poster titles* should be sent Lorenzo Margotti lorenzo.margotti3@unibo.it within December 10.

For general info please contact Daniela.Cavalcoli@unibo.it, for any help on the specific topic please contact the professor of the specific Course.

Proposed Topics

"Symmetries, electrons and phonons" (prof Boscherini)

1) *Molecular symmetries.* Describe and illustrate the symmetry operations forming the point group of selected molecules; report and discuss the character table of the corresponding point group. A useful web resource is http://symmetry.otterbein.edu/gallery/. There are numerous molecular graphics applications which can be used to make professional figures of molecular structures, including jmol (http://jmol.sourceforge.net/) and VESTA (https://jp-minerals.org/vesta/en/).
2) *Band structures.* Describe and illustrate the band structures $E(\vec{k})$ of selected crystals, including at least one semiconductor and one metal. For each case describe the 1st Brillouin zone, highlighting the high symmetry points. For metals describe and discuss the Fermi surface. Useful web resources are http://www.xcrysden.org/doc/fermi.html and http://www.phys.ufl.edu/fermisurface/ .
3) *Experimental methods for the determination of the atomic and electronic structure.* Describe the principles, phenomenology, and main experimental aspects of (choose one): 1) scattering of x-rays, neutrons or electrons to determine the atomic structure of condensed matter; or 2) photoemission to determine the electronic structure.

"Magnetism and Superconductivity" (prof Sanna)

4) *Adiabatic demagnetization and magnetocaloric materials* Describe and illustrate the principle of the adiabatic demagnetization and its application. Describe both the physical principles and how a real apparatus works by considering also an important field of application, for example:
    a. How to achieve low temperatures with paramagnetic salts and/or nuclear demagnetization.
    b. The use of ferromagnetic materials as best candidates for the fabrication of next-generation environment-friendly magnetic refrigerators and energy-related applications of magnetocaloric materials.
5) *Permanent magnets* Describe the quantum physical laws and properties which allow to have hard magnets. Discuss the most important hard ferromagnetic materials nowadays available and their applications considering possible strategies to improve their physical characteristics to satisfy energetic and environmental needs.
6) *Magnetic resonance spectroscopies* Describe the principles of one magnetic resonance technique and how it can be used to study magnetic or superconducting properties of materials.
7) *Production of high magnetic fields.* Describe how magnetic fields are produced, considering both permanent and electro-magnets, and how the record strong fields of several tens of Tesla can be achieved in hybrid conventional-superconducting magnets. Consider also some use of strong magnetic field for research or technological applications.

"Laboratory of Condensed Matter Physics" (prof Fraboni)

8) *Experimental apparatus for material characterization.* Choose one of the experimental characterization techniques illustrated in the course, based either on photon or particle probes (electrons, protons etc.) Describe and illustrate the principles of the technique. Design the experimental apparatus needed to implement such a technique and describe the peculiarities of each chosen building block. If possible, provide an estimate of the cost of the whole apparatus.
9) *Material growth methods.* Choose one of the material growth/fabrication methods illustrated in the course, based either on the top-town or bottom-up approach. Describe and illustrate the principles

of the technique. Select a recent scientific paper published in one of the following Journals: Nature Materials, Nature Nanotechnology, Nature Photonics, and critically analyze and comment the pros and cons of the selected growth/fabrication method.

“Semiconductor Materials and Nanostructures” (prof Basiricò)

10) *Feynman Lecture* “There is a lot of room at the bottom… In this famous lecture given in 1959 R Feynman proposed several possible applications of nanomaterials https://pdfs.semanticscholar.org/1bc8/21e55e3b381eaba62bb02c861b9cb5273309.pdf. Many of these applications have been done after more than 50 years, please, describe an example from the relevant scientific literature.
11) *Low dimensions in semiconductor physics*. New and interesting physical properties (optical, electronic..) arise when a semiconductor goes to “nano”. Please describe a relevant example (material or device) selected from the recent literature (review papers preferred).
12) *Advanced Functional Materials*. the unique properties of organic-hybrid small molecules and polymers, such as their easy processability from solution, the possibility of deposition at low temperature, over large areas, and by means of low-cost techniques compatible with roll-to-roll printing processes, make them ideal candidates for the development of a novel platform for advanced opto- and microelectronic devices and sensing systems, easily scalable from laboratory to industrial prototypes. Please describe an example of the possible application of such a novel technology emphasizing pros and cons with respect to the traditional one.

“Microscopic Kinetics and Thermodynamics” (Prof Pasquini)

13) *Thermoelectric materials.* Thermoelectric phenomena are an illuminating example of the symmetry of transport properties. Thermoelectric materials have a high technological importance in energy conversion and harvesting and in sensing applications. After illustrating the basic principles of thermoelectricity, describe an energy-related application of thermoelectric materials. Possibly discuss the atomic-level structure or nanostructure of a thermoelectric material of current interest. *(In addition to the course material, a review articles of thermoelectric materials is available for students interested in addressing this topic).*
14) *Atomic diffusion in nanostructures.* Describe the driving forces and fluxes that govern matter transport via diffusion in materials with a compositional gradient, illustrating the relevant atomistic mechanisms. Discuss one or two applications of these physical principles to the realization of nanostructures with peculiar morphologies, such as hollow and core-shell nanoparticles, in the light of recent (21st century!) research articles. *(A couple of examples are already available in the course material)*
15) *Nucleation phenomena in (nano) materials.* Underline the principles of nucleation theory as the key to understand a wide class of discontinuous transformations in materials. Discuss a prominent example of nucleation in traditional materials science (e.g. precipitation, solidification, shape memory effect) or in nanoscience (e.g. growth of nanoparticles from the vapor, formation of nanostructures on surfaces)

“Computational Material Physics” (Prof Franchini)

16) *Numerical solution of the Schrödinger equation for atoms and molecules.* Describe how to solve the Schrödinger equation for the He atom and for the He2 molecule using Density Functional Theory and/or the Hartree-Fock method following the variational self-consistent procedure discussed in the class. Run the given code and discuss the results. Optional: write and discuss your own code.
17) *The pseudopotential method.* Discuss the main principles and technical construction of the pseudopotential method and compute the band structure of Si and Ge following the prescription

given in Cohen & Bergstresser, Phys. Rev. 141, 789 (1966). Run the given code and discuss the results. Optional: write and discuss your own code.

18) *Electronic bandstructure using VASP*. Compute the bandstructure of a metal (simple metal like fcc Li and/or fcc Cu) and an insulator (Silicon or Diamond) using the Vienna ab initio simulation package (VASP) within Density Functional Theory and hybrid functionals. Describe the computational protocol from input to output and visualize the results. Optional: plot the Fermi surface of the selected metallic solids.