

Università degli Studi di Genova – Istituto Italiano di Tecnologia

**Corso di Dottorato “Scienze e tecnologie della chimica dei Materiali”  
Curriculum “Nanochemistry”**

Anno Accademico 2019-2020

Ciclo XXXV

<https://unige.it/en/students/phd-programmes>

**Development of new materials for energy related applications.**

*Tutor: Liberato Manna, Luca de Trizio*

The research activity will be aimed at synthesizing and characterizing semiconductor nanocrystals, with applications in energy conversion. Devices of interests are, for example, solar cells, which allow for the direct conversion of the solar energy into electrical power, thus generating “green” energy. Also, light emitting diodes (LEDs), which are the most efficient light sources, have the potential to strongly lower the consumption of electricity required for both indoor and outdoor lighting, as they use at least 75% less energy than incandescent lighting.

Colloidal semiconductor nanocrystals (NCs) have been shown as promising materials for low-cost and high efficiency solar cells and LED devices thanks to their unique properties as well as simple and safe solution phase syntheses and film fabrication. This research activity will be first focused in the synthesis of nanocrystals, including for example metal halide perovskites, metal chalcogenides and chalcogenides. In particular metal chalcogenide materials with a cubic/orthorhombic perovskite structures which have been recently demonstrated to have interesting optical properties. Such materials will be engineered in order to optimize their optical and electrical properties. Possible strategies are the encapsulation of nanocrystals in proper inorganic shells (with the formation of nano heterostructures), ligand and/or ion exchange procedures.

**Requirements:** The ideal candidate must have a Master Degree in one of the following areas: Material Science, Chemistry, Chemical Engineering or Physics.

For further details concerning the research theme, please contact: liberato.manna@iit.it, luca.detrizio@iit.it

**Colloidal nanocrystals by design.**

*Tutor: Liberato Manna, Ivan Infante*

Colloidal semiconductor nanocrystals are considered prime candidates for lighting, display technology, solar cells, photodetectors and biomedical applications. These applications have taken a dramatic improvement in the last years: the record efficiency of colloidal nanocrystals solar cells has reached 13.4% and major display manufacturers like Sony and Samsung started using semiconductor nanocrystals phosphors in their display lines. In recent years, the advancement in computer technology and of the quantum chemical software to calculate molecular properties brought to the successful description of colloidal nanocrystal of experimental size, providing new insights in the chemistry of these materials. In this research activity the successful candidate will work on the development of complex Python workflows to automatize quantum chemical calculations with machine learning libraries. The idea is to browse thousands to millions of molecular precursors that can be potentially employed in the synthesis of colloidal semiconductor nanocrystals, focusing the attention especially on metal halide perovskite nanocrystals. By including realistic experimental conditions in the screening protocol, this project aims at providing an unprecedented realism in the prediction of suitable precursors, and avoid lengthy trial-and-error syntheses and redundant calculations. The best precursor candidates will be proposed to experimental colleagues that will ultimately test these structures and help in improving the screening strategy.

**Requirements:** The ideal candidate must have a Master Degree in one of the following areas: Material Science, Chemistry, Chemical Engineering or Physics. Eventually, it is also required some provable experience in Python programming language and Python libraries such as Numpy and Scipy.

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## **Top-down approach for Lithium/Sodium-ion batteries**

*Tutor: Remo Proietti Zaccaria*

We shall address the important topic of secondary energy storage devices with special attention towards lithium/sodium-ion batteries. In particular, we shall define an innovative design and fabrication approach relying on top-down fabrication techniques for the realization of Si-based/Ge-based anodes for lithium and sodium ion batteries.

The activity will be run within the micro/nano-fabrication facility of the Italian Institute of Technology by adopting standard and innovative micro/nano-fabrication solutions aiming to the realization of a top-down engineered electrode pattern. The activity will be run in collaboration with one of the institutes of the Chinese Academy of Sciences (CAS) in charge of the theoretical analysis and design.

The final goal is to develop a highly efficient electrode capable of minimizing the “dead” zones of the active material therefore pushing the cell performance as close as possible to its theoretical capacity. The choice of materials such as Si and Ge goes towards the direction of achieving an innovative electrode, both from the design and material point of view.

**Requirements:** The successful candidate will work on the electrode design (together with the colleagues of CAS) on its fabrication and electrochemical characterization. The candidates should have a background in electrochemistry, material science, chemistry or physics with possibly some experience in battery preparation and analysis. Work experience within a micro/nano-fabrication facility will be positively considered.

For further details concerning the research theme, please contact Remo Proietti Zaccaria, Email: [remo.proietti@iit.it](mailto:remo.proietti@iit.it)

## **Evaluating multimodal therapeutic effects exploiting inorganic nanoparticles on cancer stem cells**

*Tutor: Teresa Pellegrino*

Novel inorganic heterostructures that can merge photo-ablation and magnetic hyperthermia or radiotherapy and magnetic hyperthermia is a research line that is currently being largely expanded at IIT. The objectives of this PhD thesis will focus on the study of heterostructures' biocompatibility, interactions with serum proteins, molecular and physical tumor targeting. Furthermore, cellular/tumor heat-mediated damages that occur upon photo irradiation, magnetic hyperthermia, radiotherapy or through a combination of these therapeutic approaches will be studied. Cellular studies will be conducted using 2D and 3D in vitro models (the latter of which involves cancer stem cells derived from patients). The aims of this project are to characterize the effects of multimodal therapeutic nanoplatforms on cancer stem cells derived by patients, evaluating the therapeutic effects not only on the whole tumor spheroids but also on the non-proliferating cancer stem cells, on the progenitor and on the most differentiated cancer cells. If required, involvement in in vivo animal studies will be also pursued. Requisites:

**Requirements:** We are seeking candidates with a medical or biological background that are keen to take part in an interdisciplinary project, working at the interface between biology and material science, developing skills in the field of nano-biotechnology. Knowledge of bio-molecular techniques such as real time polymerase chain reactions, immunofluorescent techniques, transfection protocols, flow cytometry, immunoprecipitation methods, stem cell culture, and in vivo animal studies is needed. Knowledge of nanoparticle characterization techniques such as dynamic light scattering, gel electrophoresis, elemental analysis thermo-gravimetric analysis is also desirable.

The candidate will be a member of a multidisciplinary team of chemists, biologists, physicists and engineers. At IIT, state-of-the-art chemistry and biology laboratories for material preparation, cellular culturing and characterization, as well as a full-equipped animal facility, are available.

For further details concerning the research theme, please contact: [teresa.pellegrino@iit.it](mailto:teresa.pellegrino@iit.it)

**Heterostructures based on upconverting nanoparticles for multiple purposes.**

Upconverting nanoparticles (UCNPs) are nanoparticles mainly known for their photon up-conversion that enables to convert incident infrared light into visible light emission. This feature makes them appealing for bio-imaging. By tuning the dopants composition it is possible to tune the emission light color as well as to introduce dopant acting as T1-contrast agents ions within the UCNP structures. We are also working on the UCNP to perform post-transformation of these nanoparticles and introduce radioisotopes. The aim of this project is to develop inorganic hetero-structures composed of at least two distinct domains, one magnetic and one based on UCNPs that will be used to merge magnetic hyperthermia, thanks to the magnetic nanoparticles, with radiotherapy or magnetic hyperthermia with T1 contrast imaging in magnetic resonance imaging.

**Requirements:** The ideal PhD with a preferable background in material science and chemistry will develop new skills on the synthesis, material characterization and post synthesis manipulation of such inorganic heterostructures, including post structural transformation (such as intercalation reaction). Also as a part of his/her research the candidate will develop procedure for water transfer and stabilization in saline media and surface modification of these nanoparticles to make the nano-heterostructures specific towards bio-molecular targets associated to cancer or for sorting and detection applications. The candidate will be a member of a multidisciplinary team of chemists, biologists, physicists and engineers. At IIT, state-of-the-art chemistry and a full equipped material characterization facility is available together with biology laboratory for in vitro and in vivo characterizations.

For any further information please refer to [teresa.pellegrino@iit.it](mailto:teresa.pellegrino@iit.it)