Annual Report - 1st PhD Year

Nicolò Petrini (XXXVI cycle)

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Zero-dimensional (0D) $Sn:In_2O_3$ (ITO) nanoparticles in colloidal solution are able to store electrons after UV light photodoping thanks to the presence of a hole-acceptor in solution. It has been recently demonstrated that the liquid hole-acceptor can be substituted by a suitable 2D material that performs an analogous role [1]. The 0D-2D material coupling is hence able to permanently store charges after light absorption, acting as a nanocapacitor system. However, further investigation is needed to find a solution for effectively extracting the charges from the nanocapacitor system to be employed as an electric source.

The final aim of my PhD project is the development of an all-solid-state device capable of storing permanently photo-generated charges and that can be employed, on demand, as an electric source, based on this 0D-2D hybrid structure.

During the first PhD year, my research activity focused on the study of core-shell nanoparticles of ITO (Indium Tin Oxide) and 2D materials. Within this framework, during the current year, I deepened my knowledge on both the 0D and the 2D systems, in order to be able in the next year to fabricate a device for the charge extraction. In particular, I can divide my activity in three main research lines:

1. **The study of the nanoparticle electronic structure and its effect on the optical properties**. We firstly implemented a model in COMSOL Multyphysics that solves the Poisson equation in the static case, taking into account the geometry of the nanoparticles and the band structures of ITO and In_2O_3. The result we achieved is the equilibrium band profile and the radial position-dependent carrier density, which highlights a depletion zone at the surface of the nanoparticles. We studied experimentally the optical response of different size core-shell ITO- In_2O_3 nanoparticles synthetized in our group. We found evidence that it is fundamental to take into account the electronic structure and the depletion region shown by the finite element model simulation for a correct understanding of evolution of the optical absorption spectrum with size and after different photo-excitation time. Part of these results have been recently submitted [2] and we are working on the publication of a more detailed analysis of the model used to fit experimental data.
2. **The fabrication of 2D materials**. MoS_2 monolayer can work as a hole-acceptor, which allows the photodoping process in the 0D – 2D system. We focused on reproducing a new technique [3] able to obtain large-area defectless 2D material flakes. This technique consists of mechanically exfoliate an ultraflat crystal of transition metal dichalcogenides (TMDC) with a previously fabricated gold tape. The chemical affinity between gold and the TMDC surface favors the breaking of weak Van der Waals forces between the TMDC layers and allows picking a single layer of the desired material, which is then deposited on a specific substrate. We were able to obtain large area MoS_2 flakes, which will be used for the subsequent device phase. Exfoliation of other composite materials has been studied too, with encouraging results both for TMDCs (MoSe, WS_2, Bi_2Te_3) and Janus monolayers (BiTeI, BiTeBr, BiTeCl). Optical characterization of these latter materials is still ongoing.
3. **Fabrication of nanoparticles films**. We recently started the fabrication of ITO- In_2O_3 nanoparticles that were dispersed in different solvents and spin coated on glass substrates in order to obtain a connected monolayer of nanocrystals. Spin coating parameters (ramp acceleration, speed, solution dilution) were optimized for each solvent to obtain a monolayer with uniform distribution of

nanocrystals. The same procedure will be performed on MoS_2 monolayer and the photodoping of the 0D-2D will be optically verified before starting to fabricate the electrodes for the final device.

Eventually, I took part in the setup of the new micro-Raman and micro-photoluminescence spectroscopic system present in the Spectroscopy Laboratory. Particularly, I helped programming the movement of the µm-resolution stepper motor stage to obtain spatially resolved micro-Raman and micro-PL maps.

Courses attended

Course	Teachers	PhD Course	Status
Materials characterization	M. Prato (IIT), L. Pasquale (IIT), S. Dante (IIT), L. Ceseracciu (IIT), M. Salerno	IIT	Passed
Optical properties of nanomaterials	D. Baranov (IIT)	IIT	Passed
Transmission electron microscopy: basics and applications to materials science and life science	1 R. Brescia (IIT), J. Buha (IIT), R. Marotta (IIT), D. Debellis (IIT) YES	IIT	Passed
Optoelectronics of nanomaterials	I. Kriegel (IIT), D. Baranov (IIT), F. Di Stasio (IIT)	IIT	Passed
Introduction to Nanophotonics and Nanofabrication	Maria Caterina Giordano	UniGe	Passed
Optical Microscopy at the Nanoscale	Alberto Diaspro	UniGe	In progress
Elementary electronic structure of solids	L. Manna (IIT)	IIT	To be done

Schools and seminars:

- Seminar "Organic and hybrid solar cells", February 23rd and 24th, 2021: Online
- VIU PhD Academy "Plastic Pollution and Bioplastic Materials", September 26th to October 1st, 2021: in presence

Publications:

Manuscript submitted for review:

"Control of electronic band profiles through depletion layer engineering in core-shell nanocrystals," M. Ghini, N. Curreli, M. B. Lodi, N.Petrini, M. Wang, M. Prato, A. Fanti, L. Manna, I. Kriegel , *Submitt. to Nat. Comm., arXiv2108.12681*, Aug. 2021

References

[1] I. Kriegel *et al.*, "Light-Driven Permanent Charge Separation across a Hybrid Zero-Dimensional/Two-Dimensional Interface," *J. Phys. Chem. C*, vol. 124, no. 14, pp. 8000–8007, 2020, doi: 10.1021/acs.jpcc.0c01147.

[2] M. Ghini *et al.*, "Control of electronic band profiles through depletion layer engineering in core-shell nanocrystals," *Submitt. to Nat. Comm., arXiv2108.12681*, Aug. 2021, [Online]. Available: http://arxiv.org/abs/2108.12681.

[3] F. Liu *et al.*, "Disassembling 2D van der Waals crystals into macroscopic monolayers and reassembling into artificial lattices," *Science (80-.).*, vol. 367, no. 6480, pp. 903–906, 2020, doi: 10.1126/science.aba1416.