First Year Report

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Research Activity

My PhD project is focused on the correlation of spectroscopy and microscopy data, along with the development of computational tools for their analysis. To achieve this, I have undertaken various projects aimed at comprehending the nature of the data under scrutiny and exploring various computational techniques.

Electron microscopy techniques offer exceptional resolution, while spectroscopy techniques provide a higher signal-to-noise ratio.

During the first year I acquired fundamental knowledge of programs and Python scripts used to process Transmission electron microscopy (TEM) and Scanning Transmission electron microscopy (STEM) (1) data, such as Hyperspy (2) and Lumispy (3). I applied these tools to extract valuable information.

I conducted characterizations on various samples of 2D materials and nanomaterials, each possessing intriguing optoelectronic properties.

Amongst two-dimensional transition metal dichalcogenides, molybdenum disulfide (**MoS_2**) raises interest because of its properties, that includes a tunable bandgap, high electron mobility and significant on/off current ratios (4) (5).

Combining **MoS2** with transparent indium thin oxide (**ITO**) creates a metallic-semiconducting interface (figure 1A). Cathodoluminescence (CL) can be employed to discern material composition and the presence of defects, while photoluminescence (PL) is useful for studying optoelectronics properties, such as the emission wavelength.

Working with a postdoc, Andrea Griesi, I applied Principal Component Analysis (PCA) and Non-negative Matrix Factorization (NMF) decomposition on the collected data to distinguish the individual exciton contributions within the signal. To identify emission peaks, I processed the data and fitted it with Gaussian curve.

Another class of materials of interest is lead halide perovskites, with applications spanning lasers, light emitting diodes, and photodetectors.

Electron Energy Loss Spectroscopy (EELS) is employed in electron microscopy to analyze these materials. By measuring peak intensities at specific energy levels, we can gain insights into material characteristics.

Hereafter, I conducted research on Cesium lead bromide (**$PbCsBr_3$**) sample growth on silicon (Si) substrates (Figure 2B), analyzing the EELS signal to measure the bandgap in various regions of the sample. The bandgap is determined by the onset of the first energy loss edge. I applied two techniques to obtain precise bandgap measurements: the first involved fitting the first derivative, while the second utilized lines interpolation.

Additionally, I applied two denoising techniques, Singular Value Decomposition (SVD) and Blind Source Separation (BSS), useful to identify the major sources of the signal.

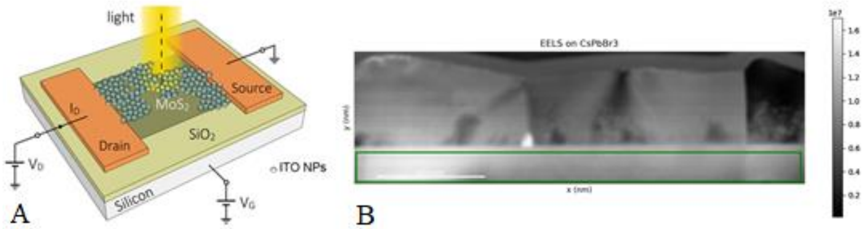

Figure 1. MoS2 with ITO nanoparticles (A) and PbCsBr3 growth on Si (B)

MXene or 2D metal carbides and nitrides were also the subject of my research due to their electromagnetic (EM) shielding properties, which find applications in electronic device fabrication to eliminate EM interference. I collected data from two MXene samples, **Ti2C3** and **TiC2**, and conducted Photoluminescence and Raman Spectrum measurements to explore their plasmonic properties. (6)

I collected data from this class of samples. I worked with two samples Ti_2C_3 and TiC_2. I measured the Photoluminescence and the Raman Spectrum, to understand the plasmonic properties.

Furthermore, I collected Raman Spectra data from eight samples of Graphene powder and attempted to infer to infer structural information from peak's ratio (7).

Served as another focal point of my research, I concentrated on developing a **machine learning** (**ML**) architecture to identify nanocrystals of $CsPbI_3$ (figure 2). I trained a convolutional neural network (CNN) with High-angle annular dark-field (HAADF) imaging and subsequently tested its ability to distinguish nanocrystals from the background. The CNN adopted a **U-Net** architecture (figure 3), encoding and decoding images to identify key features defining objects within them. This architecture has the potential to efficiently process vast amounts of data from electron microscopy experiments or detect specific regions within nanostructures.

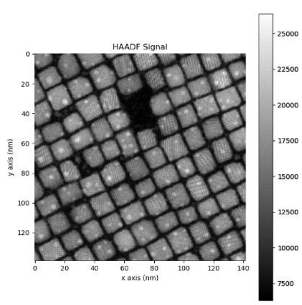

Figure 2. HAADF image of CsPbI3 nanocrystals

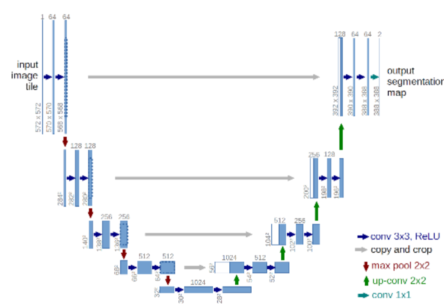

Figure 3. U-net architecture

In conclusion, my first-year experiences enhanced my programming skills, particularly in the domain of ML architecture development, while deepening my understanding of the chemistry and physics underlying nano- and 2D materials. I also focused on data collection, specifically Raman Spectra. I believe that the interdisciplinary environment of my PhD program holds promise for the development of innovative material characterization techniques.

Attended course and exams given

- **Optics for Microscopy and Spectroscopy**, held by Alessandro Zunino and Eli Slenders;
- **Advanced Electron Microscopy for Materials Science**, held by Giorgio Divitini, Rosaria Brescia, Iurii Ivanov, Andrea Griesi;
- **Machine Learning for Particle Physics**, held by Andrea Coccaro and Francesco Di Bello;
- **Chemometrics and Experimental Design**, held by Riccardo Leardi
- **BIOMED-AI Summer School: Biomedicine and Bioethics Supporting Responsible Innovation in the era of Big Data and AI**, held in Athens

List of Publications

- Resources and tools for rare disease variant interpretation, May 2023, Frontiers Molecular Biosciences (8). This publication comes from my previous research activity.

List of conference presentations

- Poster presented in Nanoinnovation2023 conference, held in Rome from 18 to 22 of September

References

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7. **Ferrari, A., Basko, D.** Raman spectroscopy as a versatile tool for studying the properties of graphene. *Nature Nanotech.* 2013, Vol. 8.

8. **Licata L, Via A, Turina P, et al.** Resources and tools for rare disease variant interpretation. *Front Mol Biosci.* May 10, 2023.