GREGORI LUCA

University of Perugia, Italy

EDUCATION

Ph.D. Candidate in Chemical Sciences nov 2020 - Present

University of Perugia

Curriculum: Theoretical Chemistry and Computational Modelling

Master's degree in chemical sciences oct 2018 – jul 2020

University of Perugia

Curriculum: Theoretical Chemistry and Computational Modelling

Erasmus+ Mobility feb 2020 – apr 2020

Universidad Autonoma de Madrid

Bachelor's degree in chemistry sep 2015 – sep 2018

University of Perugia

RESEARCH EXPERIENCE

Graduate Researcher, University of Perugia nov 2020 - Present

Advisors: **Filippo De Angelis, Daniele Meggiolaro**
Project: "Optoelectronic Properties and Defect Chemistry of Metal Halide Perovskites: Enhancing Solar Cell Stability and Efficiency"

Visiting Student, KAUST, Saudi Arabia feb 2022 – July 2022
Advisor: **Derya Baran**
Project: "Dissociative Host-Dopant Bonding Facilitates Molecular Doping in Halide Perovskites"

M.Sc. Thesis, University of Perugia feb 2022 – jul 2022

Advisors: **Filippo De Angelis, Cristina Diaz**
Title: "Reactive scattering of O2 on Cu(111): Ab Initio Molecular Dynamics Study"

Erasmus+ Period Internship, Universidad Autonoma de Madrid feb 2020 – apr 2020

Advisor: **Cristina Diaz**

Project: "Reactive scattering of O2 on Cu(111): Ab Initio Molecular Dynamics Study"

B.Sc. Thesis, University of Perugia mar 2018 – sep 2018

Advisor: **Paola Belanzoni**
Title: "Bond analysis and ligand effect in [LAu(III)Alkyne]+/2+ complexes: a theoretical approach"

PUBLICATIONS

1. Zhou, Y., van Laar, S.C., Meggiolaro, D., **Gregori, L.**, Martani, S., Heng, J.Y., Datta, K., Jiménez-López, J., Wang, F., Wong, E.L. and Poli, I., **2023**. How Photogenerated I2 Induces I-rich Phase Formation in Lead Mixed Halide Perovskites.

Advanced Materials, p.2305567.

2. Berger, F.J., Poli, I., Aktas, E., Martani, S., Meggiolaro, D., **Gregori, L.**, Albaqami, M.D., Abate, A., De Angelis, F. and Petrozza, A., 2023. How Halide Alloying Influences the Optoelectronic Quality in Tin-Halide Perovskite Solar Absorbers. *ACS Energy Letters*, 8, pp.3876-3882.

3. Lanzetta, **L., Gregori**, L., Hernandez, L.H., Sharma, A., Kern, S., Kotowska, A.M., Emwas, A.H., Gutiérrez-Arzaluz, L., Scurr, D.J., Piggott, M. and Meggiolaro, D., 2023. Dissociative Host-Dopant Bonding Facilitates Molecular Doping in Halide Perovskites. *ACS Energy Letters*, *8*, pp.2858-2867.

4. Meggiolaro, D., **Gregori, L.** and De Angelis, F., **2023**. Formation of a Mixed Valence Sn3F8 Phase May Explain the SnF2 Stabilizing Role in Tin-Halide Perovskites*. ACS Energy Letters*, 8, pp.2373-2375.

5. Martani, S., Zhou, Y., Poli, I., Aktas, E., Meggiolaro, D., Jiménez-López, J., Wong, E.L., **Gregori, L**., Prato, M., Di Girolamo, D. and Abate, A., **2023**. Defect Engineering to Achieve Photostable Wide Bandgap Metal Halide Perovskites. *ACS Energy Letters*, *8*, pp.2801-2808.

6. Kahmann, S., Meggiolaro, D., **Gregori, L**., Tekelenburg, E.K., Pitaro, M., Stranks, S.D., De Angelis, F. and Loi, M.A., 2022. The Origin of Broad Emission in⟨ 100⟩ Two-Dimensional Perovskites: Extrinsic vs Intrinsic Processes. *ACS Energy Letters*, *7*(12), pp.4232-4241.

7. Aktas, E., Pudi, R., Phung, N., Wenisch, R., **Gregori, L**., Meggiolaro, D., Flatken, M.A., De Angelis, F., Lauermann, I., Abate, A. and Palomares, E., **2022**. Role of Terminal Group Position in Triphenylamine-Based Self-Assembled Hole-Selective Molecules in Perovskite Solar Cells. *ACS Applied Materials & Interfaces*.

8. Jeong, W.H., Yu, Z., **Gregori, L**., Yang, J., Ha, S.R., Jang, J.W., Song, H., Park, J.H., Jung, E.D., Song, M.H. and Park, S.H., **2021**. "In-situ Cadmium Surface Passivation of Perovskite Nanocrystals for Blue LEDs". *Journal of Materials Chemistry A.*

9. Canil, L., Salunke, J., Wang, Q., Liu, M., Köbler, H., Flatken, M., **Gregori, L**., Meggiolaro, D., Ricciarelli, D., De Angelis, F. and Stolterfoht, M., **2021**. "Halogen-Bonded Hole-Transport Material Suppresses Charge Recombination and Enhances Stability of Perovskite Solar Cells". *Advanced Energy Materials*.

10. Mahata, A., Meggiolaro, D., **Gregori, L**. and De Angelis, F., **2021**. "Suppression of Tin Oxidation by 3D/2D Perovskite Interfacing." *The Journal of Physical Chemistry C*.

11. Caprioglio, P., Cruz, D., Caicedo-Davila, S., Zu, F., Sutanto, A.A., Pena-Camargo, F., Kegelmann, L., Meggiolaro, D., **Gregori, L**., Wolff, C.M. and Stiller, B., **2021**. "Bi-functional Interfaces by Poly-Ionic Liquid Treatment in Efficient pin and nip Perovskite Solar Cells". *Energy & Environmental Science*.

12. **Gregori, L**., Sorbelli, D., Belpassi, L., Tarantelli, F. and Belanzoni, P., **2019**. "Alkyne Activation with Gold (III) Complexes: A Quantitative Assessment of the Ligand Effect by Charge-Displacement Analysis". *Inorganic chemistry*, 58(5).

PRESENTATIONS

Talk "Dissociative Host-Dopant Bonding Facilitates Molecular Doping in Halide Perovskites". 6th International Conference on Perovskite Solar Cells and Optoelectronics" (Oxford, 18-20 September 2023)

Poster "Dissociative Host-Dopant Bonding Facilitates Molecular Doping in Halide Perovskites"
"13th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics, (Assisi 2022)

Poster "Dissociative Host-Dopant Bonding Facilitates Molecular Doping in Halide Perovskite"
XLIX Italian Conference of Inorganic Chemistry - INORG2023 (Perugia, Italy, sep 2022)

TEACHING EXPERIENCE

Teaching assistant - General and Inorganic Chemistry II (Bachelor's Degree Program at the University of Perugia, code: GP000250) for the Academic Years 2021-2022 and 2022-2023

PERSONAL SKILLS

Mother tongue(s): **Italian**

Other language(s): **English**

UNDERSTANDING		SPEAKING		WRITING
Listening	Reading	Spoken interaction	Spoken production	
B2	B2	B2	B2	B2

Levels: A1/A2: Basic user - B1/B2: Independent user - C1/C2 Proficient user

Common European Framework of Reference for Languages

JOB RELATED SKILLS

Computational Modelling

- Knowledge of Density Functional Theory and Advanced electronic structure methods.
- Experienced in using quantum chemistry software for materials science such as Quantum Espresso, VASP, CP2K, CRYSTAL leading to publication in high impact journal.
- Expertise in modelling semiconductor for optoelectronic devices and creation of interfaces to study more complexed systems.
- Use of software as Avogadro, Gnuplot, Molden, Chemdraw, Qtiplot, OriginLab to analyze structure and create input for different software.
- basic knowledge of quantum chemistry softwares Gaussian, Dalton,Orca
- basic knowledge of the classical molecular dynamics code dl_poly

Machine Learning

- Background in Machine Learning and Artificial Intelligence.
- Implemented machine learning algorithms such as linear regression or more complexes analysis such us classification of big database.
- Experience in Feature engineering, Model training, ML approach in materials science problems
- Familiar with popular frameworks python based: Tensorflow, PyTorch and Scikit-Learn.
- Skills include data preprocessing, model training, and evaluation.

Data Analysis and Visualization

- Proficient in data analysis techniques that lead to high impact journal publications.
- Utilized tools such as Python (pandas, Numpy) for data manipulation and analysis.
- Developed and implemented data visualization strategies for clear presentation of results especially with Juptyer-Notebook and Spyder software.

Operating Systems

- Proficient in Linux (Ubuntu, CentOS)
- Command line navigation, system administration, shell scripting.
- Experience with package management and software deployment on Linux environments.

- Experience in managing servers for computational tasks.
- Troubleshooting and resolving issues related to Linux systems, ensuring optimal performance.
- Implemented and managed batch processing systems for efficient job execution and resource utilization.
- Familiarity with job queuing systems like Slurm and Torque for high-performance computing environments.

High-Performance Computing (HPC)

- Managed and maintained computational clusters for efficient data calculations.
- Experience in high-performance computational chemistry resources such as clusters of computational nodes based on Intel Simple/Multicore with around 1600 CPU divided into three different and separated rack.
- Experience in parallel computing techniques for accelerated calculations.
- Basic expertise in Layer 2 and Layer 3 network protocols, including Ethernet, Infiniband, and TCP/IP.
- Basic knowledge of POSIX Operating System (LINUX) and batch system as (Torque/MAUI).
- Basic knowledge in private networking, Gigabit local network to keep worldwide connection between external laboratories vias a GARR 10 gigabits links.

COMPUTER SKILLS

SELF-ASSESSMENT

Information Processing	Communication	Content Creation	Safety	Problem Solving
Proficient User	Independent User	Independent User	Independent User	Proficient User

Levels: Basic user - Independent user - Proficient user

- Good command of Windows and Linux based operating systems.
- Good knowledge of Microsoft Office and Libre Office suites.
- Moderate knowledge of Fortran programming language.
- Basic knowledge of Adobe Suite Package (Photoshop, Illustrator, Lightroom, Premiere).
- Basic knowledge of Blender for 3D modelling and visualization.