

PERSONAL INFORMATION

Luca Gregori



Sex ____ | Date of birth ____/1996 | Nationality ____

ACTUAL POSITION

PhD Student in Chemical Sciences, XXXVITH cycle, University of Perugia
Curriculum: Theoretical Chemistry and Computational Modelling;
Research project: "Structural, electronic and optical properties of perovskite metal halide: The role of the central metal (Ge, Sn, Pb)".

Supervisor: Prof. Filippo De Angelis, Dott. Daniele Meggiolaro.

EDUCATION AND TRAINING

09/2018-07/2020

Master's Degree in Chemical Sciences (*Curriculum: Inorganic Chemistry*) - Joint European Master in Theoretical Chemistry and Computational Modelling
 Final Mark: 110/110 *cum laude*.

University of Perugia, Italy - Universidad Autonoma de Madrid, Spain
Thesis Title: "Reactive scattering of O2 on Cu(111): Ab Initio Molecular Dynamics Study"

02/2020-04/2020

Erasmus Traineeship

Madrid, Spain

Hosting Institution: Universidad Autonoma de Madrid*Supervisor:* Prof. Cristina Diaz

09/2015-09/2018

First Level Degree in Chemistry

Final Mark: 110/110.

University of Perugia, Italy

Thesis Title: "Bond analysis and ligand effect in [LAu(III)Alkyne]⁺² complexes: a theoretical approach"

09/2010-07/2015

High School with specialization in Science

Final Mark: 78/100.

"Galileo Galilei" High School, Terni, Italy

PERSONAL SKILLS

Mother tongue(s)

Italian

Other language(s)

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
English	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

- good knowledge of quantum chemistry softwares *Quantum Espresso, VASP, CRYSTAL*
- good knowledge of *Avogadro, Gnuplot, Molden, Chemdraw, Qtiplot, OriginLab* softwares
- basic knowledge of quantum chemistry softwares *Gaussian, Dalton*
- basic knowledge of the classical molecular dynamics code *dl_poly*

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.
- Good knowledge of *shell* scripting.
- Moderate knowledge of *Fortran* programming language.
- Basic knowledge of *R* and *Python* programming languages.
- Basic knowledge of *Inkscape* vector graphics editor
- Basic knowledge of Adobe Suite Package (Photoshop Illustrator Lightroom Premiere)
- Basic knowledge of Blender for 3D modelling and visualization

ADDITIONAL INFORMATION

ISI Publications

1. Aktas, E., Pudi, R., Phung, N., Wenisch, R., **Gregori, L.**, Meggiolaro, D., Flatken, M.A., De Angelis, F., Lauermaann, 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*.
2. 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*.
3. 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*.
4. 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*.
5. 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*.
6. **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).