

# Curriculum Vitae

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## Valeria Butera

Scienze e Tecnologie Biologiche Chimiche e Farmaceutiche

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### Academic Career

**March 2023** – Present: Assistant Professor (RTDa) in Inorganic Chemistry at the University of Palermo, Italy.

**April 2019 – February 2023:** Academic Researcher at Epitaxial Materials and Nanostructures, Central European Institute of Technology, CEITEC, Brno, Czech Republic.

**2016 – March 2019: Postdoctoral Fellow in Computational Chemistry** at Research Center for Computational Design of Advanced Functional Materials National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan.

**2015 – 2016: Postdoctoral Fellow in Computational Chemistry** at Department of Material Sciences and Engineering, Technion - Israel Institute of Technology, Haifa, Israel.

**2014 – 2015: Postdoctoral Fellow in Computational Chemistry** at Department of Environment and Earth Sciences, University of Milano-Bicocca, Milan, Italy.

**2010 – 2013: PhD in Inorganic-chemical Methodologies** at Department of Chemistry, University of Calabria, Arcavacata di Rende, Italy

*Thesis title: "Theoretical Investigation of New Materials Properties for the Storage and Release of Hydrogen and Proton Transfer in PEMFCs".*

**2008 – 2010: Master's Degree in Chemistry**, Department of Chemistry, University of Calabria, Arcavacata di Rende, Italy

*Thesis title: "Quantum-mechanical Study of the interaction between Neda- and Oxali-platin with Adenine and Guanine".* Final mark: 110/110 cum laude.

**2004 – 2007: Bachelor's Degree in Chemistry**, Department of Chemistry, University of Calabria, Arcavacata di Rende, Italy

*Thesis title: "Multifunctionals films for Solar Control".* Final mark: 107/110.

### Research Grants & Awards

Projects approved as Principal Investigator:

**2023** IS CRA-b project: "Unravelling the Molecular Basis of Mesothelin-Targeting Novel Engineered Fn3 Protein Scaffolds", granted 305.964 GPU hours on Cineca HPC.

**2023** IS CRA-c project: "Investigation of the interaction mode of engineered Fn3 proteins with mesothelin", granted 100.000 CPU hours + 10.000 GPU hours on Cineca HPC.

**2022** AKTION 2022 (Austria-Czech Republic mobility project).  
**2023** “Ru@MoS<sub>2</sub> as Single-Atom catalyst for the CO<sub>2</sub>RR”, granted 11.500 GPU nodehours and 6000 CPU nodehours on IT4Innovations National Supercomputing Center (Czech Republic).  
**2022** “Anti-Cancer Drugs Loaded on Functionalized CuO NPs”, granted 5000 GPU nodehours. IT4Innovations National Supercomputing Center (Czech Republic).  
**2022** “Gallium Nitride-based materials as promising photocatalysts for CO<sub>2</sub> reduction: a DFT study.” granted 11.806 CPU nodehours on IT4Innovations National Supercomputing Center (Czech Republic).  
**2021** “Photochemical CO<sub>2</sub> Conversion on Pure and Metal-Doped Gallium Nitride (GaN): a DFT study” granted 1.150.000 CPU corehours IT4Innovations National Supercomputing Center (Czech Republic).  
**2020** “Discovery of Novel Efficient Catalysts for CO<sub>2</sub> Capture and in Situ Utilization: DFT investigation”, granted 437.000 CPU corehours IT4Innovations National Supercomputing Center (Czech Republic).  
**2020** “CO<sub>2</sub> conversion into biofuels and fine chemicals: a DFT investigation” granted 656.000 CPU corehours IT4Innovations National Supercomputing Center (Czech Republic).  
**2019** “DFT Investigations of Functional Waveguide Materials for MIR Sensors” granted 994.000 CPU corehours IT4Innovations National Supercomputing Center (Czech Republic).  
**2014** “Pietro Bucci Medal” awarded by the Sezione Calabria of the Italian Chemical Society for the best PhD Thesis.

#### *Contribution to Editorial Board*

**2022.** Review Editor in “Organometallic Chemistry” section of “Frontiers in Chemistry” journal.  
**2022.** Review Editor in “Theoretical and Computational Chemistry” section of “Frontiers in Chemistry” journal.

#### *Teaching activities*

**2023-2024.** “General Chemistry with Exercise” course at Biology Faculty of Unipa (9 CFU, 84 hours).  
**2021-2022.** Material Modeling and Scientific Computing at CEITEC (2 ECTS, 52 hours).

#### *Professional Exchange and Workshop*

**09/2017:** “Minicourse on Machine Learning for Many-Body Physics”, San Paulo, Brazil.  
**02/2017:** Visiting Fellowship at UCLA.  
**10/2011-10/2012:** Visiting Fellowship at the Ecole Nationale Supérieure de Chimie de Paris - ENSCP-Chimie ParisTech.  
**07/2011:** Participation at “The WE-Heraeus Physics Summer School 2011”, Jacobs University, Bremen, Germany.  
**11/2010-02/2011:** Linux course, Università della Calabria.  
**04/2010-06/2010:** Visiting Fellowship at the Ecole Nationale Supérieure de Chimie de Paris - ENSCP-Chimie ParisTech.

#### *Research Project Experience*

Contributions to international research projects:

- NEDO project - Development of Innovative Catalytic Processes for Organosilicon Functional Materials (Japan)
- Marsilio-Ficino fellowship - I-CORE Solar Fuels (Israel)
- FP7 PEOPLE-2011-IRSES (Project no. 295172) New materials for hydrogen powered mobile applications (Italy)

#### *Research activity*

Advanced knowledge in the framework of Density Functional Theory (DFT) and Time-Dependent Density Functional Theory (TD-DFT), and on the usage of computational packages including Gaussian, ORCA, VASP, QuantumEspresso, AMBER and GROMACS.

*List of publications*

**Number of published publications: 31      H-index: 16**

SCOPUS

Google Scholar

*Most Relevant Conference participation*

- 1) 22nd International Winterschool on New Developments in Solid State Physics, 12-17 February 2023, Mauterndorf, Austria (poster).
- 2) 9th Symposium on Theoretical Biophysics (TheoBio2023), 16-20 July, 2023, Cetraro, Italy (poster).
- 3) 255th American Chemical Society (ACS) National Meeting, New Orleans, U.S.A., March 2018 (oral presentation).
- 4) Atlantic Basin Conference on Chemistry (ABCCChem), Cancun, Mexico, January 2018 (oral presentation).
- 5) 253rd American Chemical Society (ACS) National Meeting, San Francisco, U.S.A., April 2017 (oral presentation).
- 6) Convegno Congiunto Sicilia-Calabria, Catania, Italy, December 2014 (invited presentation).