

CURRICULUM VITAE – Maristella Alessio

PERSONAL DETAILS

Family name, First name: Alessio, Maristella
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Main topics of research

I am a theoretical and physical chemist working at the intersection of quantum chemistry, computational modeling of molecules and solids, and condensed-matter physics. My research focuses on developing new quantum chemical strategies to address large and complex systems, with applications ranging from quantum information science to heterogeneous catalysis. By bridging solid-state physics, surface science, and molecular magnetism, I aim to bridge these fields and develop innovative solutions to pressing scientific and technological challenges.

• Education and key qualifications

12/06/2018 (dissertation date): PhD (Dr. rer. nat.) in Physical and Theoretical Chemistry, Chemistry Department, Humboldt-Universität zu Berlin (HU Berlin), DE. Thesis title: Hybrid QM:QM methods for extended periodic systems. Advisor: Prof. Dr. Dr. h.c. Joachim Sauer.

2010–2012: Master in Chemistry, Chemistry Department, University of Torino, IT. Thesis title: Dispersion corrections to DFT methods for crystalline solids. Advisor: Prof. Dr. Bartolomeo Civalieri.

• Accademic appointments

09/2026–...: Assistant Professor at the Quantum Nanoscience Department, TU Delft, NL.

11/2024–10/2025: Postdoctoral fellow, Chemistry Department, KU Leuven, BE. Advisor: Prof. Dr. Daniel Escudero.

1/2022–10/2024: Marie Skłodowska-Curie Actions (MSCA) postdoctoral fellow, Chemistry Department, KU Leuven, BE. Advisor: Prof. Dr. Thomas Jagau.

05/2023–09/2023: Research visit (secondment), hosted by the Institute for Theoretical Physics, TU Wien, AT. Advisor: Prof. Dr. Andreas Grüneis.

08/2019–07/2022: Postdoctoral scholar, University of Southern California (USC), CA, USA. Advisor: Prof. Dr. Anna I. Krylov.

07/2018–06/2019: Postdoctoral scholar, Humboldt-Universität zu Berlin (HU Berlin), DE. Advisor: Prof. Dr. Dr. h.c. Joachim Sauer.

RESEARCH ACHIEVEMENTS AND PEER RECOGNITION

• Summary of publications (as of 22/09/2026)

I have published 18 peer-reviewed papers, including 6 as the first author, 6 as the corresponding author, 2 as the last author, and 11 independent of my PhD advisor's involvement. According to [Google Scholar](#), this body of work has granted 872 citations and an h-index of 12.

• Research funding

ERC Starting Grant (2025 call), awarded by the European Commission. Title: A quantum chemical approach to spins on surfaces; Amount: EUR 1 500 000.00; Role: PI/Grant holder; Timeframe & Status: to start in September 2026 (awarded).

MSCA postdoctoral fellowship, granted by the European Commission. Title: Quantum chemical design of molecular magnets; Amount: EUR 175 920.00; Role: Fellowship holder; Timeframe & Status: 2022–2024, completed.

Funded by the U.S. National Science Foundation. Title: Advanced molecular architectures for quantum information science; Role: Beneficiary through my employment in the group of Prof. Krylov at USC; Timeframe & Status: 2021–2022, completed.

Funded by the U.S. Department of Energy. Grant DE-SC0018910; Role: Beneficiary through my employment in the group of Prof. Krylov at USC; Timeframe & Status: 2019–2021, completed.

PhD IMPRS fellowship, funded by the International Max Planck Research School for Functional Interfaces in Physics and Chemistry (IMPRS-CS), Fritz Haber Institute, Berlin, DE; Role: PhD fellowship holder; Timeframe & Status: 2015–2018, completed.

- **Conference talks and lectures**

I disseminated my research findings with 21 conference talks and lectures, 11 of which were invited, across 7 countries, including Austria, Germany, Ireland, Italy, Poland, Norway, and the United States. Selected invitations: Coupled-Cluster Theory workshop in Telluride, Colorado, USA, 08/2024; International Congress of the World Association of Theoretical and Computational Chemists (WATOC), Oslo, Norway, 06/2025.

- **Scientific Software**

Software developer of the open-source [ezMagnet](#) (Ref. [9], using Python) and [MonaLisa](#) (Ref. [13], using C++) software. In 2012, I contributed to the development of the [CRYSTAL](#) code (Ref. [16]) using Fortran. Since 2021, I have also been involved in the development of the [Q-Chem](#) software, using C++.

TEACHING AND SUPERVISION EXPERIENCE

Throughout my career, I have supervised 7 Master's and 2 PhD students and have lectured courses at the bachelor and master levels on Molecular and Solid-State Modeling, Quantum Chemistry, and Group Theory. At TU Delft, I am establishing an independent research group where I supervise Master's and PhD students.

ACCADEMIC SERVICE

Reviewer for for Phys. Chem. Chem. Phys., Chem. Comm., J. Mater. Chem. C, J. Chem. Theory Comput. (30 verified peer reviews) and for the Swiss National Science Foundation (SNSF) and the National Science Center of Poland (NCN) (2 grant reviews).

Associate editor for Frontiers in Catalysis, Topic: “Modelling the complexity of heterogeneous catalytic materials for energy storage and conversion”, with one paper independently edited: [DOI:10.3389/fctls.2022.935174](#).

Organizer of the workshop “From Models to Reality” at Schloss Ringberg am Tegernsee, Max Planck Society, DE; 19.02–23.02; 50 participants.

Member of the YouReCa (Young Researchers' Careers, 2023–present) association at KU Leuven and of the WiSE (Women in Science and Engineering, 2019–2022) association at USC.

Reader for three Master's Theses, KU Leuven, 2022–2026.

CAREER BREAKS and DIVERSE CAREER PATHS

10/2025–08/2026: Career break due to maternity leave.

09/2019: Diverse career paths. Over the course of my career, I have actively engaged with the international research community. A pivotal moment occurred in September 2019 when I moved from Germany to California, shifting my focus from solid-state chemistry and catalysis to molecular magnetism. Despite the challenges of expanding my research expertise during the pandemic, this period soon became highly productive, characterized by innovative software developments, multiple publications, and the attainment of a MSCA fellowship.