Curriculum Vitae

Mario BARBATTI

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Research field

Theoretical, computational chemistry applied to molecular photochemistry. Method development, software implementation, and investigations of nonadiabatic processes. Mixed quantum-classical dynamics simulations. Leading developer of the Newton-X program.

Contact

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Professional Appointments

Since Sep 2015	Professor of Chemistry, Aix Marseille University, France
Sep 2010 - Aug 2015	Group Leader, Max-Planck-Institut für Kohlenforschung, Mülheim, Germany
Nov 2003 - Aug 2010	Senior scientist, Institute for Theoretical Chemistry, University of Vienna, Austria

Honors and Awards

- Senior member of the *Institut Universitaire de France*, 2021-2026
- ERC Advanced Grant, 2019-2024
- Chair of excellence A*Midex, 2015-2019

Education and Titles

2008	Habilitation for teaching Theoretical Chemistry, University of Vienna
1997 - 2001	Doctor of Sciences (Physics). Institute of Physics, Federal University of Rio de Janeiro
1995 - 1997	Master of Sciences (Physics). Institute of Physics, Federal University of Rio de Janeiro
1991 - 1995	Bachelor of Sciences (Physics), Institute of Physics, Federal University of Rio de Janeiro

Bibliographic Indicators

- Peer-reviewed papers: 159
- Book chapters: 8
- Citations: 8664 – H-index: 51
- ORCID: orcid.org/0000-0001-933 6-6607
- Research ID: F-5647-2014
- Full publication list at www.barbatti.org/publications

Selected Publications

- Barbatti, M. Simulation of Excitation by Sunlight in Mixed Quantum-Classical Dynamics. *J. Chem. Theory Comput.* **2020**, *16*, 4849-4856.
- Crespo-Otero, R.; Barbatti, M. Recent Advances and Perspectives on Nonadiabatic Mixed Quantum-Classical Dynamics. *Chem. Rev.* **2018,** *118*, 7026-7068.
- Dral, P. O.; Barbatti, M.; Thiel, W. Nonadiabatic Excited-State Dynamics with Machine Learning. *J. Phys. Chem. Lett.* **2018,** *9*, 5660-5663.
- Barbatti, M.; Ruckenbauer, M.; Plasser, F.; Pittner, J.; Granucci, G.; Persico, M.; Lischka, H. Newton-X: a surface-hopping program for nonadiabatic molecular dynamics. *WIREs: Comp. Mol. Sci.* **2014,** *4*, 26-33.
- Barbatti, M. Photorelaxation Induced by Water-Chromophore Electron Transfer. *J. Am. Chem. Soc.* **2014**, *136*, 10246-10249.

Software Development

- M. Barbatti, G. Granucci, M. Ruckenbauer, F. Plasser, R. Crespo-Otero, J. Pittner, M. Persico, and H. Lischka, **NEWTON-X: a package for Newtonian dynamics close to the crossing seam** (2007-2020), www.newtonx.org