

## Maurizio Persico - Curriculum vitae.



- Born in Genova, Italy, 1952.
- Student of the University of Pisa and Scuola Normale Superiore (SNS), 1971/1976.
- Graduated in Chemistry (“Laurea”), with a thesis in Theoretical Chemistry, supervisor J. Tomasi, 1976.
- PhD student, SNS, 1976/1980.
- Post-Doc at the Free University of Berlin, 1980/1981.
- Researcher at the SNS, 1981/1988.
- Associate professor, University of Pisa, 1988/2000.
- Full professor, University of Pisa, since 2000.
- Head of the PhD program in Chemical Sciences, University of Pisa, 2003/2007.
- President of the BSc and Master courses in Chemistry, University of Pisa, 2011-2016.
- Director of the Department of Chemistry and Industrial Chemistry, University of Pisa, since 2016.
- Chair of the national Conference of the Presidents of BSc and Master courses in Chemistry (“ConChimica”), 2015-2016.
- Invited guest, École Normale Supérieure de Paris (1993, 1995), University of Metz (1999), Institute of Mathematics and its Applications, Minneapolis (2009).

My research is devoted mainly to the theoretical study of photochemical and photophysical phenomena. I’m the author of about 140 papers in peer-reviewed journals and book chapters, of which about 60 cosigned with foreign authors. According to JCR my papers have been cited about 7100 times (6600 without self-citations), and my H-index is 32 (as of August 2016).

My research activity has two major aspects:

1) Development of original methods and techniques in different fields of the theoretical chemistry: electronic correlation and basis sets; nonadiabatic couplings; quasi-diabatic electronic states; classical, quantum mechanical and semiclassical molecular dynamics. My research group has developed a trajectory surface hopping method for excited state dynamics simulations, based on the direct calculation of semiempirical energies and wavefunctions. The QM/MM variant of the method is apt to treat condensed phase and supramolecular systems.

2) Applications to chemical problems: predissociation of diatomic and triatomic molecules; photodissociation and photoisomerization reaction mechanisms; collisional processes; infrared multiphoton absorption and related phenomena. In the last years, the focus has been on atmospheric chemistry and on photoprocesses in condensed phase of interest in photopharmacology and in materials science.

In the last years I collaborated with several research groups, based in Brussels (VUB), Cleveland (Case Western Univ.), Frankfurt am Main (Goethe Univ.), Lubbock (Texas Tech), Madrid (Universidad Autónoma and Universidad Complutense), Modena (CNR), Aix-Marseille (Univ.), Potsdam (Univ.), Santiago de Compostela

(Univ.), Vienna (Univ.), Vigo (Univ.).

I'm presently engaged in two European programs with the same heading of "Theoretical Chemistry and Computational Modelling": the Erasmus Mundus Master and the ITN-EJD Doctorate (<https://tccm.qui.uam.es>).

I regularly act as referee for several international journals (J. Am. Chem. Soc., J. Chem. Phys., PCCP, Chem. Phys., Chem. Phys. Lett., J.Phys. Chem., Theor. Chem. Acc., etc). I've also been referee or member of evaluation committees for research funding agencies and institutions, based in Italy, Austria, Belgium, Canada, France and the EU (ERC, CECAM).

I have taught courses in Quantum Chemistry, Photochemistry, Mathematics for Physical Chemistry, Numerical Methods, and Environmental Chemistry.

### Some recent publications.

1. G. Granucci, M. Persico, A. Zocante.  
Including quantum decoherence in surface hopping.  
J. Chem. Phys. **133**, 134111/1-9 (2010)
2. T. Cusati, G. Granucci, M. Persico.  
Photodynamics and time-resolved fluorescence of azobenzene in solution: a mixed quantum-classical simulation.  
J. Am. Chem. Soc. **133**, 5109-5123 (2011)
3. P. Van Leuven, V. Cantatore, M. Persico.  
Photo-orientation of Axial Molecules.  
Phys. Chem. Chem. Phys. **14**, 1957-1964 (2012)
4. G. Granucci, M. Persico, G. Spighi,  
Surface hopping trajectory simulations with spin-orbit and dynamical couplings.  
J. Chem. Phys. **137**, 22A501/1-9 (2012)
5. F. Plasser, G. Granucci, J. Pittner, M. Barbatti, M. Persico, H. Lischka,  
Surface hopping dynamics using a locally diabatic formalism: charge transfer in the ethylene dimer cation and excited state dynamics in the 2-pyridone dimer.  
J. Chem. Phys. **137**, 22A514/1-13 (2012)
6. S. Álvarez-Barcia, J. Flores, G. Granucci, M. Persico,  
A Theoretical Study of the Chemiluminescence of the Al + H<sub>2</sub>O Reaction.  
J. Phys. Chem. A, **117**, 67-74 (2013)
7. L. Favero, G. Granucci, M. Persico,  
Dynamics of acetone photodissociation: a surface hopping study.  
Phys. Chem. Chem. Phys. **15**, 20651-61 (2013)
8. M. Barbatti, M. Ruckebauer, F. Plasser, J. Pittner, G. Granucci, M. Persico, H. Lischka,  
NEWTON-X: a surface-hopping program for nonadiabatic molecular dynamics.  
WIREs Comput. Mol. Sci. **4**, 26-33 (2014)
9. L. Martínez-Fernández, I. Corral, G. Granucci, M. Persico,  
Competing ultrafast intersystem crossing and internal conversion: A time resolved picture for the deactivation of 6-Thioguanine.  
Chem. Sci. **5**, 1336-47 (2014)
10. G. Granucci, M. Persico,  
An Overview of Nonadiabatic Dynamics Simulations Methods, with Focus on the Direct Approach versus the Fitting of Potential Energy Surfaces.  
Theoret. Chem. Acc. **133**, 1526/1-28 (2014).
11. Enrico Benassi, Giovanni Granucci, Maurizio Persico, Stefano Corni,  
Can azobenzene photoisomerise when chemisorbed on a gold surface?  
J. Phys. Chem. C **119**, 5962-5974 (2015)
12. Rui Sun, Giovanni Granucci, Amit K. Paul, Matthew Siebert, Hongliang J. Liang, Grace Cheong, William L. Hase, Maurizio Persico,  
Potential Energy Surfaces for the HBr + CO<sub>2</sub> → Br+HCO + reaction in the HBr + 2 Π<sub>3/2</sub> and 2 Π<sub>1/2</sub> spin-orbit states.  
J. Chem. Phys. **142**, 104302/1-10 (2015)

13. Lucilla Favero, Giovanni Granucci, Maurizio Persico,  
Surface hopping investigation of benzophenone excited state dynamics.  
*Phys. Chem. Chem. Phys.* **18**, 10499-10506 (2016)
14. Evgenii Titov, Giovanni Granucci, Jan Philipp Götze, Maurizio Persico, Peter Saalfrank,  
Dynamics of Azobenzene Dimer Photoisomerization: Electronic and Steric Effects.  
*J. Phys. Chem. Lett.* **7**, 3591-3596 (2016)