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, 2016-2018.
- Chair of the national Conference of the Coordinators 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 have authored about 150 papers in peer-reviewed journals and book chapters, of which about 70 cosigned with foreign authors. I am coauthor of the textbook "Photochemistry: a modern theoretical perspective" (Springer 2018). According to JCR my papers have been cited about 8300 times and my H-index is 34 (as of November 2018).

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. Distinctive features of the method are quantum decoherence corrections and the ability to treat spin-orbit and dynamic couplings on the same footing.
2) Applications to chemical problems: predissociation of diatomic and triatomic molecules, photodissociation and photoisomerization reaction mechanisms, collisional processes, infrared multiphoton absorption and strong-field phenomena. In the last years, the focus has been on photoprocesses in condensed phase of interest in molecular biology, pharmacology, materials science and photovoltaics.

In the last years I collaborated with several research groups, based in Brussels (VUB), Cleveland (Case Western Univ.), Frankfurt am Main (Goethe Univ.), Groningen (Univ.), Lubbock (Texas Tech), Madrid (Universidad Autònoma and Universidad Complutense), Modena (CNR), Aix-Marseille (Univ.), Padova (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, Czech Republic, 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. Zoccante.
   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_2O 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. Ruckenbauer, 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 2 → Br+HCO + reaction in the HBr + 2 Π 3/2 and 2 Π 1/2 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)