

Maurizio Persico - List of publications.

- [1] Renzo Cimiraglia, Maurizio Persico, Jacopo Tomasi,
The cis-trans thermal and photochemical interconversion mechanisms in the diimide N-oxide. A comparison of the results obtainable with different ab initio calculation techniques.
Chem. Phys. **24**, 251-61 (1977)
- [2] Renzo Cimiraglia, Maurizio Persico, Jacopo Tomasi,
Azoxycompounds and oxadiaziridines. An ab initio study of the ring closure reactions and of the cis-trans isomerizations.
J. Phys. Chem. **81**, 1876-82 (1977)
- [3] Renzo Cimiraglia, Maurizio Persico, Jacopo Tomasi,
Alternative paths in the ring opening of oxadiaziridine: the diimide N-oxide versus the oxodiimide rearrangement.
Theoret. Chim. Acta **49**, 13-23 (1978)
- [4] Renzo Cimiraglia, Maurizio Persico, Jacopo Tomasi,
On the direct calculation of the time evolution of excited molecular states in the presence of non adiabatic interactions.
Chem. Phys. **34**, 103-112 (1978)
- [5] Renzo Cimiraglia, Maurizio Persico, Jacopo Tomasi,
Torsional barriers and the electronic spectrum of nitrosomethane.
Chem. Phys. Lett. **63**, 352-4 (1979)
- [6] Renzo Cimiraglia, Maurizio Persico, Jacopo Tomasi,
The theoretical study of predissociation in diatomics. The case of the $O_2 B'^3\Sigma_u^-$ state.
Chem. Phys. **42**, 297-303 (1979)
- [7] Renzo Cimiraglia, Maurizio Persico,
Comments on the diabatic representation.
Mol. Phys. **38**, 1707-10 (1979)
- [8] Renzo Cimiraglia, Maurizio Persico, Jacopo Tomasi,
Roto-electronic and spin-orbit couplings in the predissociation of HNO. A theoretical calculation.
Chem. Phys. Lett. **76**, 169-71 (1980)
- [9] Renzo Cimiraglia, Maurizio Persico, Jacopo Tomasi,
The evaluation of nonadiabatic matrix elements. A comparison of different approximations applied to $LiH X - A^1\Sigma^+$.
Chem. Phys. **53**, 357-63 (1980)

- [10] Maurizio Persico,
The role of nonadiabatic coupling and sudden polarization in the photoisomerization of olefins.
J. Am. Chem. Soc. **102**, 7839-45 (1980)
- [11] Renzo Cimiraglia, Maurizio Persico,
On the $A^1\Sigma^+ - ^1\Pi$ transition in BH: Λ -doubling and vibrational structure ab initio calculations.
J. Mol. Spectry **87**, 303-11 (1981)
- [12] Vlasta Bonačić-Koutecký, Lionello Pogliani, Maurizio Persico, Jaroslav Koutecký,
Geometrical relaxation in the excited singlet states of propylene.
Tetrahedron **38**, 741-51 (1982)
- [13] Maurizio Persico, Vlasta Bonačić-Koutecký,
Nonadiabatic coupling between low lying singlet states of geometrically relaxed olefins; ethylene and propylene.
J. Chem. Phys. **76**, 6018-30 (1982)
- [14] Werner Reiland, Hans-Ulrich Tittes, Ingolf V. Hertel, Vlasta Bonačić-Koutecký, Maurizio Persico,
Stereochemical effects in the quenching of Na^* (3^2P) by CO: crossed beam experiment and ab initio CI potential energy surfaces.
J. Chem. Phys. **77**, 1908-20 (1982)
- [15] Vlasta Bonačić-Koutecký, Maurizio Persico, Detlef Döhnert, Alain Sevin,
A CI study of geometrical relaxation in the excited states of butadiene: energy surfaces and properties for simultaneous torsion and elongation of one double bond.
J. Am. Chem. Soc. **104**, 6900-907 (1982)
- [16] Vlasta Bonačić-Koutecký, Maurizio Persico,
Avoided crossing of molecular excited states and photochemistry: butadiene and unprotonated Schiff base.
Int. J. Q. Chem. **23**, 517-33 (1983)
- [17] Vlasta Bonačić-Koutecký, Maurizio Persico,
CI study of geometrical relaxation in the ground and excited singlet and triplet states of unprotonated Schiff bases: allylideneimine and formaldimine.
J. Am. Chem. Soc. **105**, 3388-95 (1983)
- [18] Renzo Cimiraglia, Maurizio Persico, Jacopo Tomasi, Oleg P. Charkin,
Electron correlation and relative energetic characteristics of complex hydrides of light elements. Part I: beryllhydrides.
J. Comput. Chem. **5**, 263-71 (1984)

- [19] Marie-Christine Bacchus-Montabonel, Renzo Cimiraglia, Maurizio Persico,
The determination of radial nonadiabatic coupling: HeNe⁺⁺ as a case study.
J. Phys. B **17**, 1931-42 (1984)
- [20] Maurizio Persico, Jacopo Tomasi,
An evaluation of solvent effects on isomerization mechanisms in diimide and
methylenimine.
Croatica Chemica Acta **57**, 1341-55 (1984)
- [21] Maurizio Persico,
Diabatic states from ab initio calculations. A new method applied to the
Na(²S,²P) + N₂ system.
in "Spectral line shapes" vol. 3, ed. F. Rostas, de Gruyter, Berlin (ISBN 3 11
010119 X), 1985, pp. 587-613
- [22] Renzo Cimiraglia, Maurizio Persico, Jacopo Tomasi,
An ab initio study of the photodissociation of nitrosoalkanes and nitrosamines.
J. Am. Chem. Soc. **107**, 1617-22 (1985)
- [23] Daniela Papierowska-Kaminski, Maurizio Persico, Vlasta Bonačić-Koutecký,
On the quenching mechanism of Na*(³P_{3/2}) by CO: surface hopping trajectory
calculations with ab initio CI potential energy surfaces.
Chem. Phys. Lett. **113**, 264-70 (1985)
- [24] Renzo Cimiraglia, Jean-Paul Malrieu, Maurizio Persico, Fernand Spiegelmann,
Quasi diabatic states and dynamical couplings from ab initio CI calculations.
A new proposal.
J. Phys. B **18**, 3073-84 (1985)
- [25] Marie-Christine Bacchus-Montabonel, Renzo Cimiraglia, Maurizio Persico,
Determination of the radial coupling between molecular states.
J. Mol. Struct. THEOCHEM **120**, 285-9 (1985)
- [26] Marie-Christine Bacchus-Montabonel, Eliane Mercier, Renzo Cimiraglia, Mau-
rizio Persico,
A non-adiabatic representation of potential energy curves. Study of the HeNe²⁺
system.
Studies in Phys. Theor. Chem. **35**, 349-55 (1985).
- [27] Renzo Cimiraglia, Maurizio Persico, Jacopo Tomasi, Oleg P. Charkin,
Electronnaja korrelazija i otnositel'nye energeticeskie charakteristiki v neem-
piriceskich rascetach kompleksnyh berillogidrirov legkich elementov
Kordinatsionnaya Khimiya **12**, 291-306 (1986)

- [28] Renzo Cimiraglia, Maurizio Persico,
Recent advances in multi-reference second order perturbation CI: the CIPSI method revisited.
J. Comput. Chem. **8**, 39-47 (1987)
- [29] Renzo Cimiraglia, Daniel Maynau, Maurizio Persico,
Simplified treatment of organic substituents in SCF-CI calculations. The methyl group.
J. Chem. Phys. **87**, 1653-60 (1987)
- [30] Hans-Jörg Hofmann, Renzo Cimiraglia, Maurizio Persico,
On the conformational structure of silabiphenyls.
Chem. Phys. Lett. **146**, 249-252 (1988)
- [31] Renzo Cimiraglia, Daniel Maynau, Maurizio Persico,
Contracted and supercontracted basis sets in the theoretical treatment of coordination compounds: the cyclopentadienyl anion and ferrocene.
Chem. Phys. Lett. **153**, 507-510 (1988)
- [32] Roberto Ambrosetti, Maurizio Persico,
ERWIN: un programma didattico per la soluzione dell'equazione di Schrödinger.
C.N.R., Progetto strategico tecnologie ed innovazioni didattiche. Note di accompagnamento del materiale prodotto (Bologna, 1988), pagg. 13-16.
- [33] Roberto Ambrosetti, Maurizio Persico,
Dall'atomo alla tavola periodica.
C.N.R., Progetto strategico tecnologie ed innovazioni didattiche. Note di accompagnamento del materiale prodotto (Bologna, 1988), pagg. 17-22.
- [34] Donatella Persico, Maurizio Persico,
a) Le leggi dei gas.
b) Separazioni.
c) BCTC.
d) Benzene.
Recensioni di programmi del progetto SERAPHIM, in "Guida all'analisi del software didattico", a cura di G. Olimpo, M. Ott, C.N.R. e Istituto Geografico De Agostini (Novara, 1989, ISBN 88-402-0319-2), pagg. 45-53.
- [35] Maurizio Persico
Approssimazione di Born-Oppenheimer ed accoppiamenti vibronici.
in "Scuola di Chimica Teorica, Torino 13-23/9/1989. Basi teoriche ed applicazioni numeriche.", a cura di R. Moccia, C. Pisani, Polo Editoriale Chimico (Milano, 1990), pagg. 101-128.

- [36] Maurizio Persico, Ivo Cacelli, Alessandro Ferretti,
The photodissociation of dimethylnitrosamine studied by classical trajectories
on ab initio potential energy surfaces.
J. Chem. Phys. **94**, 5508-23 (1991)
- [37] Maurizio Cossi, Maurizio Persico,
Charge transfer and curve crossings in the $[\text{Be H}_2\text{O}]^{2+}$ system.
Theoret. Chim. Acta **81**, 157-168 (1991)
- [38] Marco Clericuzio, Carlo Rosini, Maurizio Persico, Piero Salvadori,
About the origin of the chiroptical properties of the planar diene chromophore
in cyclohexylidenepropene derivatives.
J. Org. Chem. **56**, 4343-46 (1991)
- [39] Marino Cavazza, Renzo Cimiraglia, Maurizio Persico, Francesco Pietra, Maur-
izio Zandomenoghi,
Changes in electronically excited states and photochemistry of troponoids on
complexation with acids.
J. Photochem. Photobiol. A **61**, 329-342 (1991)
- [40] Lorenzo Di Bari, Maurizio Persico, Carlo Alberto Veracini,
The problem of coupled internal rotations in substituted ethoxybenzenes: max-
imum entropy analysis of LX-NMR data and ab initio rotameric distributions.
J. Chem. Phys. **96**, 4782-91 (1992)
- [41] Giovanni Granucci, Maurizio Persico,
Electronic structure, vibrational spectrum and photochemistry of the $\text{Fe} + \text{H}_2$
system.
Chem. Phys. **167**, 121-130 (1992)
- [42] Franca Floris, Maurizio Persico, Alessandro Tani, Jacopo Tomasi,
Ab initio effective pair potentials for simulations of the liquid state, based on
the polarizable continuum model of the solvent.
Chem. Phys. Lett. **199**, 518-524 (1992)
- [43] Roberto Bianco, Stanislav Miertuš, Maurizio Persico, Jacopo Tomasi,
Molecular reactivity in solution. Modelling of the effects of the solvent and of
its stochastic fluctuation on the S_N2 reaction.
Chem. Phys. **168**, 281-292 (1992)
- [44] Manuel Aguilar, Roberto Bianco, Stanislav Miertuš, Maurizio Persico, Jacopo
Tomasi,
Chemical reactions in solution. Modelling of the delay of solvent synchronism
(dielectric friction) along the reaction path of a S_N2 reaction.
Chem. Phys. **174**, 397-407 (1993)

- [45] Giovanni Granucci, Maurizio Persico,
Electronic structure of compounds with Fe-C bonds.
J. Mol. Struct. THEOCHEM **283**, 111-116 (1993)
- [46] Giovanni Granucci, Maurizio Persico,
Benzene-O₂ interaction potential from ab initio calculations.
Chem. Phys. Lett. **205**, 331-336 (1993)
- [47] Jan Broeckhove, Bernd Feyen, Piet Van Leuven, Renzo Cimiraglia, Maurizio Persico,
Quantum wavepacket dynamics on the BH $^1\Sigma^+$ states.
J. Phys. B **26**, 4471-4482 (1993)
- [48] Jan Broeckhove, Bernd Feyen, Piet Van Leuven, Renzo Cimiraglia, Maurizio Persico,
Quantum wavepacket dynamics for the $^1\Sigma^+$ states of boron hydride.
Int. J. Quantum Chem. S **27**, 517-526 (1993)
- [49] Maurizio Persico,
Tunnelling in the $A^1\Pi$ state and the dissociation energy of BH.
Mol. Phys. **81**, 1463-71 (1994)
- [50] Maurizio Cossi, Maurizio Persico, Jacopo Tomasi,
A simple solvent model for electron transfer reactions.
J. Mol. Liquids **60**, 87-105 (1994)
- [51] Maurizio Cossi, Maurizio Persico, Jacopo Tomasi,
Aspects of electrophilic bromination of alkenes in solution. Theoretical calculation of atomic charges in bromonium ions.
J. Am. Chem. Soc. **116**, 5373-78 (1994)
- [52] Franca Maria Floris, Maurizio Persico, Alessandro Tani, Jacopo Tomasi,
Hydration shell structure of the calcium ion from simulations with ab initio effective pair potentials.
Chem. Phys. Lett. **227**, 126-132 (1994)
- [53] Jacopo Tomasi, Maurizio Persico,
Molecular interactions in solution: an overview of methods based on continuous distributions of the solvent.
Chem. Rev. **94**, 2027-2094 (1994)
- [54] Maurizio Persico
Ab initio methods in computational chemistry.
in "Approaches to Structure-Property Relationship", ed. G. Bolis, M. Botta e A. Martinelli, Tipografia Senese (Siena, 1995)

- [55] Celestino Angeli, Giuseppe Del Re, Maurizio Persico,
Quasi-bond orbitals from maximum-localization hybrids for ab initio CI calculations.
Chem. Phys. Lett. **233**, 102-110 (1995)
- [56] Franca Floris, Maurizio Persico, Alessandro Tani, Jacopo Tomasi,
Free energies and structures of hydrated cations, based on effective pair potentials.
Chem. Phys. **195**, 207-220 (1995)
- [57] Celestino Angeli, Maurizio Persico, Maria Allegrini, Giuseppe De Filippo, Francesco Fuso, Dieter Gruber, Laurentius Windholz, Maurizio Musso,
Theoretical analysis of the emission spectra of the NaCd excimer.
J. Chem. Phys. **102**, 7782-88 (1995)
- [58] Giovanni Granucci, Maurizio Persico,
Coherent excitation of wavepackets in two electronic states. Interference effects at an avoided crossing.
Chem. Phys. Lett. **246**, 228-234 (1995)
- [59] Maurizio Persico, Renzo Cimiraglia, Fernand Spiegelmann,
An ab initio study of the lowest $1,3\Sigma^+$ states of BH. Quasi diabatic curves and vibronic couplings.
in "Strategies and Applications in Quantum Chemistry", p. 349-365, ed. Y. Ellinger e M. Defranceschi, Kluwer Acad. Press (Dordrecht, 1996, ISBN 0-7923-3837-5)
- [60] Maurizio Persico, Piet Van Leuven,
Multiphoton absorption and anharmonicity.
Phys. Rev. A **53**, 366-372 (1996)
- [61] Celestino Angeli, Maurizio Persico,
Quasi-diabatic and adiabatic states and potential energy curves for Na-Cd collisions and excimer formation.
Chem. Phys. **204**, 57-64 (1996)
- [62] Alessandro Ferretti, Giovanni Granucci, Alessandro Lami, Maurizio Persico, Giovanni Villani,
Quantum mechanical and semiclassical dynamics at a conical intersection.
[J. Chem. Phys. **104**, 5517-27 \(1996\)](#)
- [63] Celestino Angeli, Giovanni Granucci, Maurizio Persico,
A surface hopping study of energy transfer in Na + Cd* collisions.
Chem. Phys. Lett. **255**, 65-70 (1996)

- [64] Sylvie Magnier, Maurizio Persico, Naseem Rahman,
Bound-bound and bound-free $X^2\Sigma_g^+ \rightarrow A^2\Pi_u$ transitions in Na_2^+ relevant for
experiments in Above Threshold Dissociation.
Chem. Phys. Lett. **262**, 747-750 (1996)
- [65] Paola Cattaneo, Maurizio Persico,
Ab initio determination of quasi-diabatic states for multiple reaction pathways.
Chem. Phys. **214**, 49-60 (1997)
- [66] David Romstad, Giovanni Granucci, Maurizio Persico,
Nonadiabatic transitions and interference in photodissociation dynamics.
Chem. Phys. **219**, 21-30 (1997)
- [67] Piet Van Leuven, Maurizio Persico,
Multiphoton absorption and rotation: a model study.
J. Phys. B **30**, 1503-16 (1997)
- [68] Sylvie Magnier, Celestino Angeli, Giovanni Granucci, Françoise Masnou-
Seeuws, Maria Allegrini, Maurizio Persico,
Theoretical study of $\text{Na}(4p^2P)+\text{Na}(3s^2S)$ and $\text{Cd}(5p^3P_0)+\text{Na}(3s^2S)$ collisions
and their role in the energy transfer between Cd^* and Na .
Z. Phys. D **39**, 261-265 (1997)
- [69] Sylvie Magnier, Maurizio Persico, Naseem Rahman,
Quantum wavepacket dynamics simulations of Above Threshold Dissociation in
 Na_2^+ .
Chem. Phys. Lett. **279**, 361-366 (1997)
- [70] Paola Cattaneo, Maurizio Persico,
Wavepacket dynamics in the presence of a conical intersection.
J. Phys. Chem. A **101**, 3454-60 (1997)
- [71] Maurizio Persico, Piet Van Leuven,
Short-time quantum dynamics of the driven rigid rotor.
Z. Phys. D **41**, 139-142 (1997)
- [72] Celestino Angeli, Renzo Cimiraglia, Maurizio Persico, Alessandro Toniolo,
Multireference perturbation CI I: extrapolation procedures with CAS or se-
lected zero-order spaces.
Theoret. Chem. Acc. **98**, 57-63 (1997) .
- [73] Celestino Angeli, Maurizio Persico,
Multireference perturbation CI II: selection of the zero-order space.
Theoret. Chem. Acc. **98**, 117-128 (1997)

- [74] Maurizio Persico,
Electronic diabatic states: definition, computation and applications.
in "The Encyclopedia of Computational Chemistry", ed. P. v. R. Schleyer, N.
L. Allinger, T. Clark, J. Gasteiger, P. A. Kollman, H. F. Schaefer III, P. R.
Schreiner, J. Wiley (Chichester, 1998, ISBN 04-7196-588-X), vol. 2, pp. 852-
860
- [75] Piet Van Leuven, Maurizio Persico,
Multiphoton absorption and phase correlation between driving field and molec-
ular dipole.
J. Phys. B **31**, 2903-19 (1998)
- [76] Paola Cattaneo, Maurizio Persico,
Semiclassical treatment of the photofragmentation of azomethane.
Chem. Phys. Lett. **289**, 160-166 (1998)
- [77] Celestino Angeli, Renzo Cimiraglia, Maurizio Persico,
Multireference perturbation CI III: Fast evaluation of the one-particle density
matrix.
Theoret. Chem. Acc. **100**, 324-328 (1998)
- [78] Paola Cattaneo, Giovanni Granucci, Maurizio Persico,
Simulations of condensed phase photochemistry: cage effect and internal con-
version in azoalkanes and nitrosamines.
J. Phys. Chem. A **103**, 3364-3371 (1999)
- [79] Sylvie Magnier, Maurizio Persico, Naseem Rahman,
Above Threshold Dissociation and wavepacket propagation.
Laser Physics **9**, 403-406 (1999)
- [80] Paola Cattaneo, Maurizio Persico, Alessandro Tani,
Nonadiabatic dynamics in solution: MD and surface hopping.
Chem. Phys. **246** 315-322 (1999)
- [81] Sylvie Magnier, Maurizio Persico, Naseem Rahman,
Rabi oscillations between dissociative molecular states.
[Phys. Rev. Letters **83**, 2159-62 \(1999\)](#)
- [82] Paola Cattaneo, Maurizio Persico,
An ab initio study of the photochemistry of azobenzene.
Phys. Chem. Chem. Phys. **1**, 4739-43 (1999)
- [83] Marco Malvaldi, Maurizio Persico, Piet Van Leuven,
Infra-red multiphoton absorption and electronic polarizability.
[J. Chem. Phys. **111**, 9560-67 \(1999\)](#)

- [84] Sylvie Magnier, Maurizio Persico, Naseem Rahman,
Theoretical study of two-photon above threshold dissociation and related processes in Na_2^+ and Li_2^+ .
[J. Phys. Chem. A **103**, 10691-98 \(1999\)](#)
- [85] Paola Cattaneo, Maurizio Persico,
Diabatic and adiabatic potential energy surfaces for azomethane photochemistry.
Theoret. Chem. Acc. **103**, 390-398 (2000)
- [86] Alessandro Toniolo, Maurizio Persico, Demetrio Pitea,
An ab initio study of spectroscopy and predissociation of ClO.
[J. Chem. Phys. **112**, 2790-97 \(2000\)](#)
- [87] Marie-Christine Bacchus-Montabonel, Dahbia Talbi, Maurizio Persico,
Quantum chemical determination of the rate coefficients for radiative association of CH_3^+ and H_2 .
J. Phys. B **33**, 955-959 (2000)
- [88] Alessandro Toniolo, Maurizio Persico, Demetrio Pitea,
Theoretical photoabsorption spectra for ClOOC1 and Cl₂O.
[J. Phys. Chem. A **104**, 7278-83 \(2000\)](#)
- [89] Fabrizio Santoro, Carlo Petrongolo, Giovanni Granucci, Maurizio Persico,
Quantum and semiclassical dynamics at the NO_2 X^2A'/A^2A' conical intersection.
[Chem. Phys. **259**, 193-200 \(2000\)](#)
- [90] Alessandro Toniolo, Maurizio Persico,
Efficient calculation of Franck-Condon factors and vibronic couplings in polyatomics.
[J. Comput. Chem. **22**, 968-975 \(2001\)](#)
- [91] Andrea Fioretti, Carlo Gabbanini, Maurizio Persico, Ivo Cacelli, Marina Mazzoni,
Line shape study of three-photon ionization through intermediate states of Rb atoms.
in "Spectral Line Shapes", vol. 11, AIP Conference Proceedings 559, 15th IC-SLS, Berlin, Germany, 10-14 July 2000), J. Seidel ed., American Institute of Physics, ISBN 1-56396-991-2 (2001), pp. 293-295.
- [92] Chiara Collaveri, Giovanni Granucci, Maurizio Persico, Alessandro Toniolo,
Theoretical study of the photochemistry of Cl₂O.
[J. Chem. Phys. **115**, 1251-1263 \(2001\)](#)

- [93] Giovanni Granucci, Maurizio Persico, Alessandro Toniolo,
Direct semiclassical simulation of photochemical processes with semiempirical wavefunctions.
J. Chem. Phys. **114**, 10608-10615 (2001)
- [94] Paola Cattaneo, Maurizio Persico,
Semiclassical simulations of azomethane photochemistry.
J. Am. Chem. Soc. **123**, 7638-7645 (2001)
- [95] Alessandro Toniolo, Maurizio Persico,
A theoretical study of spectroscopy and predissociation dynamics in nitrosoalkanes.
J. Chem. Phys. **115**, 1817-1827 (2001)
- [96] Maurizio Persico, Piet Van Leuven,
On the mechanism of infrared multiphoton absorption by diatomic molecules in intense laser fields.
Physicalia Magazine **23**, 21-35 (2001)
- [97] Alessandro Toniolo, Giovanni Granucci, Silvia Inglese, Maurizio Persico,
Theoretical study of the photodissociation dynamics of ClOOC1.
Phys. Chem. Chem. Phys. **3**, 4266-4279 (2001)
- [98] Giovanni Granucci, Sylvie Magnier, Maurizio Persico,
Rabi oscillations in the dissociative continuum: rotation and alignment effects.
J. Chem. Phys. **116**, 1022-1029 (2002)
- [99] Piet Van Leuven, Marco Malvaldi, Maurizio Persico,
Infra-red multiphoton absorption and alignment of diatomic molecules in a continuous wave field.
J. Chem. Phys. **116**, 538-546 (2002)
- [100] Ivo Cacelli, Andrea Fioretti, Carlo Gabbanini, Marina Mazzoni, Maurizio Persico,
Line shape study of two-color three-photon ionization of Rb atoms.
Phys. Rev. A **66**, 639-648 (2002)
- [101] Maurizio Persico, Giovanni Granucci, Silvia Inglese, Teodoro Laino, Alessandro Toniolo,
Semiclassical simulation of photochemical reactions in condensed phase.
J. Mol. Struct. THEOCHEM **621**, 119-126 (2003)
- [102] Elio Napolitano, Vittorio Farina, Maurizio Persico,
The Stille reaction: a density functional theory analysis of the transmetalation and the importance of coordination expansion at tin.
Organometallics **22**, 4030-4037 (2003)

- [103] Giuliano Alagona, Caterina Ghio, Maurizio Persico, Simone Tomasi,
Quantum mechanical study of stereoselectivity in the oxazaborolidine-catalyzed
reduction of acetophenone.
[J. Am. Chem. Soc. **125**, 10027-10039 \(2003\)](#)
- [104] Alessandro Toniolo, Cosimo Ciminelli, Giovanni Granucci, Teodoro Laino,
Maurizio Persico,
QM/MM connection atoms for the multistate treatment of organic and biological
molecules.
[Theoret. Chem. Acc. **93**, 270-279 \(2004\)](#)
- [105] Maurizio Persico,
Jacopo Tomasi.
[Theoret. Chem. Acc. **93**, 58-60 \(2004\)](#)
- [106] Cosimo Ciminelli, Giovanni Granucci, Maurizio Persico,
The photoisomerization mechanism of azobenzene: a semiclassical simulation
of nonadiabatic dynamics.
[Chem. Eur. J. **10**, 2327-2341 \(2004\)](#)
- [107] Giovanni Granucci, Maurizio Persico, Piet Van Leuven,
Alignment of molecules in pulsed resonant laser fields.
[J. Chem. Phys. **120**, 7438-7445 \(2004\)](#)
- [108] Enrique Bustos, Giovanni Granucci, Maurizio Persico, Ana M. Velasco, In-
maculada Martín, Carmen Lavín,
A Theoretical Study for the Valence-Rydberg Interaction in Diatomic
Molecules. Application to the NO β Band System.
[J. Phys. Chem. A **108**, 11279-11284 \(2004\)](#)
- [109] Mario Barbatti, Giovanni Granucci, Maurizio Persico, Hans Lischka,
Semiempirical molecular dynamics investigation of the excited state lifetime of
ethylene.
[Chem. Phys. Lett. **401**, 276-281 \(2005\)](#)
- [110] Silvia Inglese, Giovanni Granucci, Teodoro Laino, Maurizio Persico,
Photodissociation dynamics of chlorine peroxide adsorbed on ice.
[J. Phys. Chem. B **109**, 7941-7947 \(2005\)](#)
- [111] Giovanni Granucci, Marina Mazzoni, Maurizio Persico, Alessandro Toniolo,
A computational study of the excited states of bilirubin IX.
[Phys. Chem. Chem. Phys. **7**, 2594-2598 \(2005\)](#)
- [112] Emilio Martínez-Núñez, Saulo Vázquez, Giovanni Granucci, Maurizio Persico,
Carlos M. Estevez,

- Photodissociation of formic acid. A trajectory surface hopping study.
Chem. Phys. Lett. **412**, 35-40 (2005)
- [113] Marina Mazzoni, Giovanni Agati, Maurizio Persico, Riccardo Pratesi,
A spectroscopic study of wavelength dependent photoisomerizations of bilirubins in aqueous solution bound to HSA.
J. Opt. A: Pure Appl. Opt. **7**, 742-747 (2005)
- [114] Cosimo Ciminelli, Giovanni Granucci, Maurizio Persico,
Are azobenzenophanes rotation-restricted?
J. Chem. Phys. **123**, 174317/1-10 (2005)
- [115] Alessandro Toniolo, Cosimo Ciminelli, Maurizio Persico, Todd J. Martínez,
Simulation of the photodynamics of azobenzene on its first excited state: comparison of full multiple spawning and surface hopping treatments.
J. Chem. Phys. **123**, 234308/1-10 (2005)
- [116] Piet Van Leuven, Maurizio Persico,
Rotational averaging and optimization of laser-induced population transfer in molecules.
J. Chem. Phys. **124**, 054319/1-13 (2006)
- [117] Pietro Amat, Giovanni Granucci, Francesco Buda, Maurizio Persico, Valentina Tozzini,
The chromophore of asFP595: a theoretical study.
J. Phys. Chem. B **110**, 9348-9353 (2006)
- [118] Giovanni Granucci, Maurizio Persico,
Excited state dynamics with the direct trajectory surface hopping method: azobenzene and its derivatives as a case study.
Theoret. Chem. Acc. **117**, 1131-1143 (2007)
- [119] Mario Barbatti, Giovanni Granucci, Maurizio Persico, Matthias Ruckebauer, Mario Vazdar, Mirjana Eckert-Maksić, Hans Lischka,
The on-the-fly surface-hopping program system NEWTON-X: application to ab initio simulation of the nonadiabatic photodynamics of benchmark systems.
J. Photochem. Photobiol. A **190**, 228-240 (2007)
- [120] Giovanni Granucci, Maurizio Persico,
A critical appraisal of the fewest switches algorithm for surface hopping.
J. Chem. Phys. **126**, 134114/1-11 (2007)
- [121] Giovanni Granucci, Maurizio Persico,
Photochemistry in condensed phase.

in “Continuum Solvation Models in Chemical Physics: from Theory to Applications”, R. Cammi and B. Mennucci eds., ISBN 978-0-470-02938-1, J. Wiley (2007), pp. 450-470.

- [122] Luigi Creatini, Teresa Cusati, Giovanni Granucci, Maurizio Persico, Photodynamics of azobenzene in a hindering environment. *Chem. Phys.* **347**, 492-502 (2008)
- [123] Cosimo Ciminelli, Giovanni Granucci, Maurizio Persico, The photoisomerization of a peptidic derivative of azobenzene: a nonadiabatic dynamics simulation of a supramolecular system. *Chem. Phys.* **349**, 325-333 (2008)
- [124] Teresa Cusati, Giovanni Granucci, Maurizio Persico, Gloria Spighi, Oscillator strength and polarization of the forbidden $n \rightarrow \pi^*$ band of *trans*-azobenzene. A computational study. *J. Chem. Phys.* **128**, 194312/1-9 (2008)
- [125] Maurizio Persico, Piet Van Leuven, Photo-orientation of molecules on a surface. *Phys. Chem. Chem. Phys.* **11**, 8433-39 (2009)
- [126] Patricia Hurd, Teresa Cusati, Maurizio Persico, Trajectory integration with potential energy discontinuities. *J. Comp. Phys.* **229**, 2109-2116 (2010)
- [127] Ana M. Velasco, Carmen Lavín, Enrique Bustos, Inmaculada Martín, Giovanni Granucci, Maurizio Persico, Absorption Oscillator Strengths for Vibronic Transitions of $np\pi$ Rydberg Series in NO. *J. Phys. Chem. A* **114**, 8450-8456 (2010)
- [128] Giovanni Granucci, Maurizio Persico, Alberto Zoccante, Including quantum decoherence in surface hopping. *J. Chem. Phys.* **133**, 134111/1-9 (2010)
- [129] Teresa Cusati, Giovanni Granucci, Maurizio Persico, Photodynamics and time-resolved fluorescence of azobenzene in solution: a mixed quantum-classical simulation. *J. Am. Chem. Soc.* **133**, 5109-5123 (2011)
- [130] Kyoyeon Park, Joshua Engelkemier, Maurizio Persico, Paranjothy Manikandan, William L. Hase, Algorithms for Sampling a Quantum Microcanonical Ensemble of Harmonic Oscillators at Potential Minima and Conical Intersections. *J. Phys. Chem. A* **115**, 6603-09 (2011)

- [131] Giovanni Granucci, Maurizio Persico,
Gradients for Configuration Interaction energies with Spin-Orbit coupling in a semiempirical framework.
J. Comput. Chem. **32**, 2690-96 (2011)
- [132] Teresa Cusati, Giovanni Granucci, Emilio Martínez-Núñez, Francesca Martini, Maurizio Persico, Saulo Vázquez,
Semiempirical hamiltonian for simulation of azobenzene photochemistry.
J. Phys. Chem. A **116**, 98-110 (2012)
- [133] Piet Van Leuven, Valentina Cantatore, Maurizio Persico,
Photo-orientation of Axial Molecules.
Phys. Chem. Chem. Phys. **14**, 1957-1964 (2012)
- [134] Valentina Cantatore, Giovanni Granucci, Maurizio Persico,
Stochastic model for photoinduced anisotropy.
J. Comput. Chem. **33**, 1015-1022 (2012), DOI: 10.1002/jcc.22931
- [135] Giovanni Granucci, Maurizio Persico, Gloria Spighi,
Surface hopping trajectory simulations with spin-orbit and dynamical couplings.
J. Chem. Phys. **137**, 22A501/1-9 (2012)
- [136] Felix Plasser, Giovanni Granucci, Jiri Pittner, Mario Barbatti, Maurizio Persico, Hans 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)
- [137] Sonia Álvarez-Barcia, Jesús R. Flores, Giovanni Granucci, Maurizio Persico,
A Theoretical Study of the Chemiluminescence of the Al + H₂O Reaction.
J. Phys. Chem. A **117**, 67-74 (2013)
- [138] Lucilla Favero, Giovanni Granucci, Maurizio Persico,
Dynamics of acetone photodissociation: a surface hopping study.
Phys. Chem. Chem. Phys. **15**, 20651-61 (2013)
- [139] Mario Barbatti, Matthias Ruckebauer, Felix Plasser, Jiri Pittner, Giovanni Granucci, Maurizio Persico, Hans Lischka,
NEWTON-X: a surface-hopping program for nonadiabatic molecular dynamics.
WIREs Comput. Mol. Sci. **4**, 26-33 (2014), DOI: 10.1002/wcms.1158
- [140] Lara Martínez-Fernández, Inés Corral, Giovanni Granucci, Maurizio Persico,
Competing ultrafast intersystem crossing and internal conversion: A time resolved picture for the deactivation of 6-Thioguanine.
Chem. Sci. **5**, 1336-47 (2014), DOI 10.1039/C3SC52856A

- [141] Juan José Bajo, Giovanni Granucci, Maurizio Persico,
Interplay of radiative and nonradiative transitions in surface hopping with
radiation-molecule interactions.
J. Chem. Phys. **140**, 044113/1-7 (2014), DOI [10.1063/1.4862738](https://doi.org/10.1063/1.4862738)
- [142] Valentina Cantatore, Giovanni Granucci, Maurizio Persico,
Simulation of the $\pi \rightarrow \pi^*$ photodynamics of azobenzene: decoherence and
solvent effects.
Comput. Theor. Chem. **1040**, 126-135 (2014)
- [143] Giovanni Granucci, Maurizio 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).
The final publication will be available at Springer via
<http://dx.doi.org/10.1007/s00214-014-1526-1>
- [144] Valentina Cantatore, Giovanni Granucci, Maurizio Persico,
The photo-orientation of azobenzene in viscous solutions, simulated by a
stochastic model.
Phys. Chem. Chem. Phys. **16**, 25081-25092 (2014)
- [145] 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)
- [146] Rui Sun, Giovanni Granucci, Amit K. Paul, Matthew Siebert, Hongliang J.
Liang, Grace Cheong, William L. Hase, Maurizio Persico,
Potential Energy Surfaces for the $\text{HBr}^+ + \text{CO}_2 \rightarrow \text{Br} + \text{HCO}^+$ reaction in the
 $\text{HBr}^+ \ ^2\Pi_{3/2}$ and $\ ^2\Pi_{1/2}$ spin-orbit states.
J. Chem. Phys. **142**, 104302/1-10 (2015)
- [147] Lucilla Favero, Giovanni Granucci, Maurizio Persico,
Surface hopping investigation of benzophenone excited state dynamics.
Phys. Chem. Chem. Phys. **18**, 10499-10506 (2016)
- [148] 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)
- [149] Valentina Cantatore, Giovanni Granucci, Guillaume Rousseau, Giancarlo
Padula, Maurizio Persico,
Photoisomerization of Self-Assembled Monolayers of Azobiphenyls: Simulations

Highlight the Role of Packing and Defects.
J. Phys. Chem. Lett. **7**, 4027-4031 (2016)

- [150] Maurizio Persico,
La conferenza dei coordinatori di corsi di Laurea di area chimica.
Chim. Ind. **98**, 10-13 (2016)
- [151] Lara Martínez-Fernández, Giovanni Granucci, Marvin Pollum, Carlo E. Crespo-Hernández, Maurizio Persico, Inés Corral,
Decoding the molecular basis for the population mechanism of the triplet phototoxic precursors in UVA light-activated pyrimidine anticancer drugs.
Chem. Eur. J. **23**, 2619-2627 (2017)
- [152] Giovanni Granucci, Giacomo Melani, Maurizio Persico, Piet Van Leuven,
Energy Selection in Nonadiabatic Transitions.
J. Phys. Chem. A **122**, 678-689 (2018)
- [153] Padmabati Mondal, Giovanni Granucci, Dominique Rastädter, Maurizio Persico, Irene Burghardt,
Azobenzene as a Photoregulator Covalently Attached to RNA: A Quantum Mechanics/Molecular Mechanics-Surface Hopping Dynamics Study.
[Chem. Sci. **9**, 4671-4681 \(2018\)](#)
- [154] Maurizio Persico, Giovanni Granucci,
Photochemistry. A Modern Theoretical Perspective.
Part of the “Theoretical Chemistry and Computational Modelling” book series (TCCM), Springer, Cham (Switzerland), 2018
- [155] Davide Accomasso, Giovanni Granucci, Remco W. A. Havenith, Maurizio Persico,
Testing new chromophores for singlet fission: a computational protocol applied to 2,3-diamino-1,4-benzoquinone.
Submitted
- [156] Jacopo Fregoni, Giovanni Granucci, Emanuele Coccia, Maurizio Persico, Stefano Corni,
Manipulating azobenzene photoisomerization through strong light-molecule coupling.
Submitted