Pubblications

M. Alagia, N. Balucani, P. Candori, S. Falcinelli, F. Pirani, R. Richter, M. Rosi, S. Stranges, F. Vecchiocattivi
Production of ions at high energy and its role in extraterrestrial environments
Rendiconti Lincei - Scienze Fisiche e Naturali, in press; doi: 10.1007/s12210-012-0215-z

M. Alagia, C. Callegari, P. Candori, S. Falcinelli, F. Pirani, R. Richter, S. Stranges e F. Vecchiocattivi

Angular and energy distribution of fragment ions in dissociative double photoionization of acetylene molecules at 39 eV

The Journal of Chemical Physics 136 204302-1 204302-6 (2012); DOI: 10.1063/1.4720350

M. Alagia, P. Candori, S. Falcinelli, K. C. Mundim, M. S. P. Mundim, F. Pirani, R. Richter, S. Stranges e F. Vecchiocattivi

Lifetime and kinetic energy release of metastable dications dissociation

Chemical Physics 398, 134-141 (2012); DOI: 10.1016/j.chemphys.2011.03.031

A.F. Albernaz, R. Gargano, P.R.P. Barreto, N. Balucani
An extensive theoretical study for the CN + C_2H_4 reaction
IEEE Proceedings, 12th International Conference on Computational Science and Its Applications (2012) 57-62; doi:10.1109/ICCSA.2012.19

M. Albertí, A. Aguilar, J. M. Lucas, F. Pirani

Competitive role of CH_4–CH_4 and CH-π interactions in C_6H_6-$(CH_4)_n$ aggregates: the transition from dimer to cluster features

The Journal Physical Chemistry A 116, 5480-5490 (2012); DOI: 10.1021/jp3023698

M. Albertí, A. Aguilar, F. Pirani

Propensities in the solvation of M^+-benzene systems (M = Na, K, Rb) investigated by cluster dynamics

Chemical Physics 399, 290-295 (2012); DOI: 10.1016/j.chemphys.2011.07.030

M. Albertí, A. Costantini, A. Laganà, F. Pirani,
Are micelles needed to form methane hydrates in sodium dodecyl sulfate solutions?
J. Phys. Chem. B, 116 (14), 4220–4227 (2012); DOI: 10.1021/jp301124z

M. Albertí, A. Costantini, A. Laganà, F. Pirani

Are Micelles Needed to Form Methane Hydrates in Sodium Dodecyl Sulfate Solutions?,

J. Phys. Chem. B 116, 4220−4227 (2012) DOI: 10.1021/jp301124z

M. Albertí, N. Faginas Lago
Ion Size Influence on the Ar Solvation Shells of M+ −C6F6 Clusters (M = Na, K, Rb, Cs).

J. Phys. Chem. A, 116, 3094−3102 (2012), DOI.org/10.1021/jp300156k |

M. Albertí, N. Faginas Lago, F. Pirani
Benzene water interaction: From gaseous dimers to solvated aggregates.
Chemical Physics, 399, 232-239 (2012); ISSN 0301-0104, DOI:10.1016/j.chemphys.2011.08.009.

V. Aquilanti, H. M. Haggard, A. Hedeman, N. Jeevanjee, R. G. Littlejohn, L. Yu,
Semiclassical mechanics of the Wigner 6j-symbol
Journal of Physics A: Mathematical and Theoretical, 45, 065209 (2012)

N. Balucani
Elementary reactions of N atoms with hydrocarbons: first steps towards the formation of prebiotic N-containing molecules in planetary atmospheres. Chemical Society Reviews, 41 (2012) 5473-5483; doi:10.1039/C2CS35113G

N. Balucani
Nitrogen fixation by photochemistry in the atmosphere of Titan and implications for prebiotic chemistry
In: The Early Evolution of the Atmospheres of Terrestrial Planets, edited by J.M. Trigo-Rodriguez, F. Raulin, C. Muller and C. Nixon, Springer Series in Astrophysics and Space Science Proceedings, Vol. 38 (2013), in press.

N. Balucani, A. Bartocci, B. Brunetti, P. Candori, S. Falcinelli, F. Palazzetti, F. Pirani e F.

Vecchiocattivi

Collisional autoionization dynamics of $Ne^{*}(^{3}P_{2,0})$-H_2O

Chemical Physics Letters 546, 34-39 (2012); DOI: 10.1016/j.cplett.2012.07.051

N. Balucani, F. Leonori, P. Casavecchia
Crossed molecular beam studies of bimolecular reactions of relevance in combustion. Energy 43, 47-54 (2012); doi:10.1016/j.energy.2011.10.052

N. Balucani, D. Skouteris, F. Leonori, R. Petrucci, M. Hamberg, W.D. Geppert, P. Casavecchia, M. Rosi
Combined Crossed Beam and Theoretical Studies of the N(D-2) + C2H4 Reaction and Implications for Atmospheric Models of Titan
Journal of Physical Chemistry A (2012) Volume: 116(43) 10467-10479 DOI: 10.1021/jp3072316

P. R. B. Barreto, A. F. Albernaz, A. Capobianco, F. Palazzetti, A. Lombardi, G. Grossi, V. Aquilanti,
Potential energy surfaces for interactions of H_2O with H_2, N_2 and O_2: A hyperspherical harmonics representation, and a minimal model for the H_2O-rare-gas-atom systems
Computational and Theoretical Chemistry, 990, 53-61 (2012)

M. Bartolomei, F. Pirani, A. Laganà, A. Lombardi,
A full dimensional Grid empowered simulation of the CO_2 + CO_2 processes
J. Comp. Chem. (ISSN:0192-8651), 33, 1806–1819 (2012); DOI: 10.1002/jcc.23010

A. C. P. Bitencourt, A. Marzuoli, M. Ragni, R. W. Anderson, V. Aquilanti,
Exact and asymptotic computations of elementary spin networks: Classification of the quantum-classical boundaries
Lecture Notes in Computer Science, 7333, 723-737 (2012).

L. Bonnet, P. Larrégaray, V. Aquilanti,
Introduction to Jean-Claude Rayez Festschrift
Computational and Theoretical Chemistry, 990, pp. 1-2 (2012)

J. M. Bowman, D. M. Neumark, R. Welsch, R. Wester, D.J. Nesbitt, S. E. Bradforth, M. N. R. Ashfold, S. H. Kable, D. Glowacki, D. G. Truhlar, N. Balucani, A. Lagana, T.J. Martinez, A. Wodtke, T. M. Bernhardt, A. J. Orr-Ewing, R. Wester, D. Skouteris, D.W. Chandler, M. Gruebele, D.J. Nesbitt, N. Huse, S. Harris
Molecular Reaction Dynamics in Gases, Liquids and Interfaces: General Discussion. Faraday Discuss. 157, 475-500 (2012); doi: 10.1039/C2FD90014A

B. Brunetti, P. Candori, D. Cappelletti, S. Falcinelli, F. Pirani, D. Stranges e F. Vecchiocattivi
Penning ionization electron spectroscopy of water molecules by metastable neon atoms
Chemical Physics Letters 539-540, 19-23 (2012); DOI: 10.1016/j.cplett.2012.05.020

D. Calderini, S. Cavalli, C. Coletti, G. Grossi, V. Aquilanti,
Hydrogenoid orbitals revisited: From Slater orbitals to Coulomb Sturmians
Journal of Chemical Sciences, 124, 187-192 (2012)

D. Cappelletti, P. Candori, S. Falcinelli, M. Albertí, F. Pirani
A molecular beam scattering investigation of methanol – noble gas complexes: characterization of the isotropic potential and insights into the nature of the interaction
Chemical Physics Letters 545, 14-20 (2012); DOI: 10.1016/j.cplett.2012.07.020

D. Cappelletti, E. Ronca, L. Belpassi, F. Tarantelli, F. Pirani
Revealing charge-transfer effects in gas –phase water chemistry
Accounts of Chemical Research 45, 1571-1580 (2012); DOI: 10.1021/ar3000635

D.-C Che, K. Kanda, F. Palazzetti, V. Aquilanti, T. Kasai,
Electrostatic hexapole state-selection of the asymmetric-top molecule propylene oxide: Rotational and orientational distributions Chemical Physics, 399, 180-192 (2012)

.,

A. Costantini, M. Albertì, F. Pirani, A. Laganà
A Molecular Dynamics Study of Sodium Dodecyl Sulfate-Methane System in Water Using the Improved Lennard Jones formulation,

Int. J. Quantum Chem., 112 (7): 1810–1817, 2012; (ISSN:0020-7608), DOI: 10.1002/qua.23060

A. Costantini, O. Gervasi, A. Laganà
A Fault Tolerant Workflow for CPU Demanding Calculations, Lecture Notes in Computer Science, 2011, Volume 6784, 387-396 (2011) DOI: 10.1007/978-3-642-21931-3_30

A. Costantini, R. Murri, S. Maffioletti, A. Laganà
A Grid execution model for Computational Chemistry Applications using the GC3Pie framework and the AppPot VM environment
Lecture Notes Computer Science 7333, 401-416 (2012)

A. Costantini, R. Murri, S. Maffioletti, A. Laganà
A Grid execution model for Computational Chemistry Applications using the GC3Pie framework and AppPot. EGI Community Forum 2012 / EMI Second Technical Conference (2012) PoS(EGICF12-EMITC2)058. ISSN 1824-8039

O. Dutuit, N. Carrasco, R. Thissen, V. Vuitton, C. Alcaraz, P. Pernot, N. Balucani, P. Casavecchia, A. Canosa, S. Le Picard, J.-C. Loison, Z. Herman, J. Zabka, D. Ascenzi, P. Tosi, P. Franceschi, S. D. Price, P. Lavvas
Critical review of N, N^+, N_2^+, N^{++} and N_2^{++} main production processes and reactions of relevance to Titan's atmosphere. Astrophysical Journal Supplement Series, in press (doi: 10.1088/0067-0049/204/2/20).

N. Faginas Lago, A. Lombardi, A. Lagana, F. Pirani, S. Falcinelli
A bond-bond portable approach to intermolecular interactions: simulations for N-methylacetamide and carbon dioxide dimers,
Lecture Notes Computer Science 7333, 387–400 (2012).

F. Filomia, P. Saxena, C. Durante, F. De Rienzo, M. Cocchi, M. C. Menziani
Computational Insights into ADAMTS4, ADAMTS5 and MMP13 Inhibitor Selectivity.
Molecular Informatics 31, 421-430 (2012) doi: 10.1002/minf.201100131

B. Fu, Y.-C. Han, J. M. Bowman, L. Angelucci, N. Balucani, F. Leonori, P. Casavecchia
Intersystem crossing and dynamics in $O(^3P)+C_2H_4$ multichannel reaction: Experiment validates theory. PNAS (Proc. Natl. Acad. Sci. U.S.A) 109 (25) 9733-9738 (2012); doi:10.1073/pnas.1202672109

B. Fu, Y.-C. Han, J. M. Bowman, F. Leonori, N. Balucani, L. Angelucci, A. Occhiogrosso, R. Petrucci, P. Casavecchia

Experimental and theoretical studies of the $O(^3P)+C_2H_4$ reaction dynamics: Collision energy dependence of branching ratios and extent of intersystem crossing. J. Chem. Phys. 137 (22), 22A532-1 - 22A532-22 (2012); doi:10.1063/1.4746758

E. Garcia, F.J. Aoiz, A. Laganà
A classical versus quantum mechanics study of the OH + CO -> CO2 + H reaction
Theoretical Chemistry Accounts: Theory, Computation, and Modeling (Theoretica Chimica Acta), Vol. 131, No. 8. (1 August 2012), pp. 1-11, doi:10.1007/s00214-012-1262-3

E. Garcia, A. Laganà, D. Skouteris
An innovative computational comparison of exact and centrifugal sudden quantum properties of the N + N_2 reaction
Phys. Chem. Chem. Phys., 14, 1589–1595 (2012); DOI: 10.1039/C2CP22922F

A. Laganà,
The EOS start-up company,
Virt&l-Comm.1.2012.9, ISSN:2279-8773

A. Laganà,
TECHSPIN: a european network of technology spinners for sustainable innovation,
Virt&l-Comm Vol. 2, Virt&l-Comm.2.2012.1 (2012), ISSN: 2279-8773

A. Laganà,
Towards a CMMST VRC,
Virt&l-Comm.2.2012.2 (2012), ISSN: 2279-8773

A. Laganà, S. Crocchianti, G. Tentella, A. Costantini
The MPI Structure of Chimere,

Lecture Notes in Computer Science, Volume 7333/2012, 417-431, (2012) DOI: 10.1007/978-3-642-31125-3_32

A. Laganà, E. Garcia , A. Paladini, P. Casavecchia, N. Balucani,
The last mile of molecular reaction dynamics virtual experiments: the case of the OH (N=1-10) + CO (j=0-3) -> H + CO2 reaction
Faraday Discussion of Chem. Soc. 157, 415 - 436 (2012); doi: 10.1039/c2fd20046e.

A. Laganà, C. Manuali, A. Costantini, E. Rossi, M. Carpenè, A. Ghiselli, M. Cecchi,
HIPEG: a project for a High Performance Grid bridging HTC and HPC in scientific computing,
Virt&l-Comm Vol. 1, p. 10 (2012), ISSN: 2279-8773

A. Laganà, C. Manuali, S. Rampino, A. Costantini, E. Rossi, M. Carpené, A. Ghiselli, M. Cecchi,
High Performance Grid Computing: getting HPC and HTC all together, EGI Community Forum 2012 / EMI Second Technical Conference, Leibnitz Supercomputing Centre (LRZ), Munich (DE), 26-30 March 2012, Track Coordination and Communication, 144 (2012)

A. Laganà, C. Manuali, S. Rampino, A. Costantini, E. Rossi, M. Carpenè, A. Ghiselli, M. Cecchi
High Performance Grid Computing: getting HPC and HTC all together. EGI Community Forum 2012 / EMI Second Technical Conference (2012) PoS(EGICF12-EMITC2)144. ISSN 1824-8039

M. Gruebele, S. E. Bradforth, D.M. Neumark, D. G. Truhlar, M. N. R. Ashfold, D.J. Nesbitt, S. Harris, N. Huse, R. Wester, D. Glowacki, G. M. Roberts, H.H. Fielding, J.M. Bowman, Stavros, A. G. Suits, Kable, A. J. Orr-Ewing, N. Balucani, J.C. Polanyi, D. Stranges, M. P. Grubb, M. J. T. Jordan, T. J. Martinez, F. F. Crim, E. Ripani, S.J. Sibener, T.M. Bernhardt
Molecular Reaction Dynamics in Gases, Liquids and Interfaces: General Discussion. Faraday Discuss. 157, 243-264 (2012); doi: 10.1039/C2FD90012B

F. Leonori, A. Occhiogrosso, N. Balucani, A. Bucci, R. Petrucci, P. Casavecchia
Crossed Molecular Beam Dynamics Studies of the $O(^3P)$ + Allene Reaction: Primary Products, Branching ratios and Dominant Role of Intersystem Crossing. J. Phys. Chem. Letters 3, 75-80 (2012); doi.org/10.1021/jz201519q

F. Leonori, R. Petrucci, X. Wang, P. Casavecchia, N. Balucani
A crossed beam study of the reaction $CN+C_2H_4$ at a high collision energy: the opening of a new reaction channel. Chem. Phys. Lett. 553, 1-5 (2012); doi:10.1016/j.cplett.2012.09.070

F. Leonori, D. Skouteris, R. Petrucci, P. Casavecchia, M. Rosi, N. Balucani.
Combined crossed beam and theoretical studies of the C(D-1) + CH4 reaction
JOURNAL OF CHEMICAL PHYSICS, in press.

A. Lombardi, N. Faginas Lago, A. Lagana', F. Pirani, S. Falcinelli
A bond-bond portable approach to intermolecular interactions: in from gas condensed phase to simulations for N-methylacetamide and carbon dioxide
Lecture Notes Computer Science 7333, 387-400 (2012)

A. Lombardi, M. Ragni, I. F. De Fernandes,
Umbrella inversion processes. Disentanglement of the vibration-rotation problem and eigenfunctions
(2012) Proceedings - 12th International Conference on Computational Science and Its Applications, ICCSA , 6257613, 77-82 (2012).

C. Manuali, A. Costantini, A. Lagana', M. Cecchi, A. Ghiselli, M. Carpene', E. Rossi
Efficient Workload Distribution bridging HTC and HPC in Scientific Computing
Lecture Notes Computer Science 7333, 345-357 (2012)

J. M. C. Marques, J.L. Llanio-Trujillo, M. Albertí, A. Aguilar, F. Pirani

Alkali-ion microsolvation with benzene molecules

The Journal Physical Chemistry A 116, 4947-4956 (2012); DOI: 10.1021/jp302136u

L. Pacifici, D. Nalli. A. Laganà
Quantum reactive scattering calculations on GPU
Lecture Notes Computer Science 7333, 292-303 (2012)

F. Palazzetti, G. S. Maciel, A. Lombardi, G. Grossi, V. Aquilanti,
The astrochemical observatory: Molecules in the laboratory and in the cosmos
Journal of the Chinese Chemical Society, 59, 1045-1052 (2012).

M. S. Pedrosa Mundim, P. Candori, S. Falcinelli, K.C. Mundim, F. Pirani e F. Vecchiocattivi

A new statistical method for the determination of dynamical features of molecular dication dissociation processes

Lecture Notes in Computer Science, 7333, 432-446 (2012); DOI: 10.1007/978-3-642-31125-3

F. Pirani, P. Candori, M. S. Pedrosa Mundim, L. Belpassi, F. Tarantelli e D. Cappelletti

On the role of charge transfer in the stabilization of weakly bound complexes involving water and hydrogen sulphide molecules

Chemical Physics 398, 176 - 185 (2012); DOI: 10.1016/j.chemphys.2011.03.030

S. Rampino, N. Faginas Lago, A. Laganà, F. Huarte-Larranga
An Extension of the Grid Empowered Molecular Simulator to Quantum Reactive Scattering.
J. Comput. Chem. 2012, 33, 708–714 (2012); DOI: 10.1002/jcc.22878

S. Rampino, A. Laganà,
Bond Order Uniform grids for quantum reactive scattering
International Journal of Quantum Chemistry 112(7), 1818–1828 (2012), DOI: 10.1002/qua.23058

S. Rampino, A. Monari, S. Evangelisti, E. Rossi, A. Laganà
A priori modeling of chemical reactions on computational grid platforms: workflows and data models,
Chemical Physics 398, 192-198 (2012), DOI 10.1016/j.chemphys.2011.04.028

M. Rosi, P. Candori, S. Falcinelli, M. S. Pedrosa Mundim, F. Pirani, F. Vecchiocattivi

Theoretical and experimental study of the energy and structure of fragment ions produced by double photoionization of benzene molecules

Lecture Notes in Computer Science, 7333, 316-330 (2012); DOI: 10.1007/978-3-642-31125-3

M. Rosi, S. Falcinelli, N. Balucani, P. Casavecchia, F. Leonori, D. Skouteris
Theoretical study of reactions relevant for atmospheric models of Titan: interaction of excited nitrogen atoms with small hydrocarbons. Lecture Notes in Computer Science 7333, 331-344 (2012).

D. Skouteris, A. Laganà
Electronuclear MCTDH calculations on the confined H atom with mobile electron and nucleus

Int. J. Quantum Chemistry accettato DOI 10.1002/qua.24295

D. Skouteris, A. Laganà, F. Pirani,
An approximate quantum mechanical study of the N+O -> NO++e(-) associative ionisation
CHEMICAL PHYSICS LETTERS, in the press.

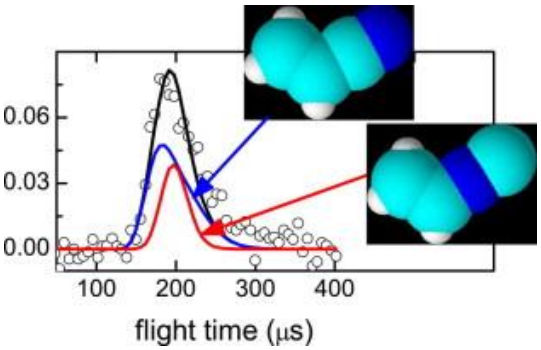
S. Tasso, S. Pallottelli, M. Ferroni, R. Bastianini, A. Laganà,
Taxonomy management in a Federation of Distributed Repositories: a chemistry use case
Lecture Notes Computer Science 7333, 358-370 (2012)

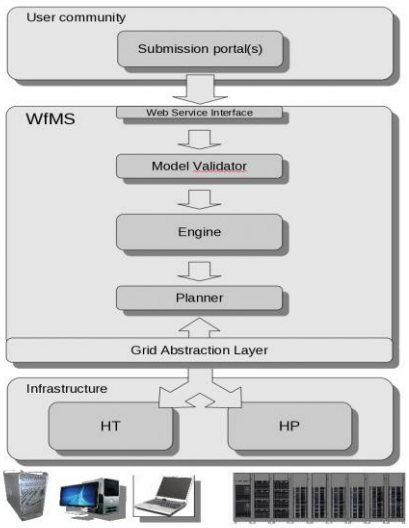
D. Truhlar, S. Sibener, J. Polanyi, D. Nesbitt, J. Bowman, D. Neumark, S. Kable, D. Glowacki, P. Casavecchia, R. Wester, A. Orr-Ewing, M. Jordan, S. Falcinelli, F. Crim, H. Vancik, K. Liu, R. Beck, A. Suits, D. Chandler, V. Aquilanti, D. Zhang, N. Balucani, D. Skouteris, M. Costes
Molecular Reaction Dynamics in Gases, Liquids and Interfaces: General Discussion. Faraday Discuss. 157, 113-140 (2012); doi: 10.1039/C2FD90011D

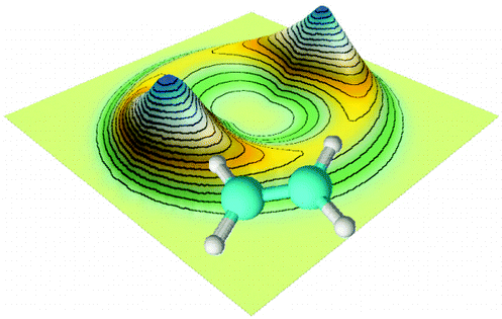
M. Verdicchio, L. Pacifici, A. Laganà,
Grid Enabled High Level Ab Initio Electronic Structure Calculations for the N_2+N_2 Exchange Reaction
Lecture Notes Computer Science 7333, 371-386 (2012)

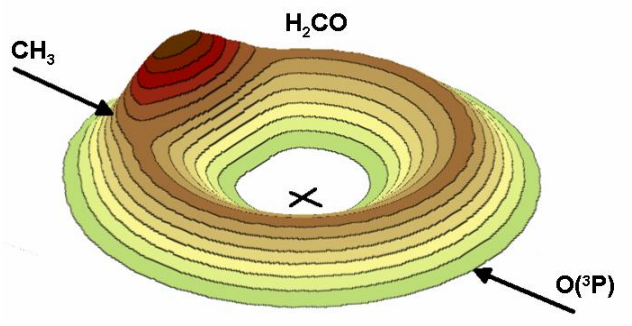
H.R.R. Vila, L.A. Leal, J.B.L. Martins, D. Skouteris, S.G. Magela, R. Gargano
The H+Li-2 bimolecular exchange reaction: Dynamical and kinetical properties at J=0
Journal of Chemical Physics 136(13), 134319 (2012) DOI: 10.1063/1.3700164

V. Vuitton, O. Dutuit, M. A. Smith, N. Balucani
Chemistry of Titan's atmosphere
In: Titan: Surface, Atmosphere and Magnetosphere, I. Mueller-Wodarg, C. Griffith, E. Lellouch & T. Cravens, Eds., Cambridge University Press, in press.








H2CO
CH3
O(3P)