CRESPOS Cédric
Birth: 25.07.1974 in Bordeaux (France)
Assistant Professor / University of Bordeaux

Education and scientific position

Since 2004	Permanent position as **assistant professor of the University of Bordeaux** Institut des Sciences Moléculaire - ISM (UMR 5255 CNRS / Université de Bordeaux)
2003 / 2004	**Temporary associate professor** (ATER) Laboratoire de Physico-Chimie Moléculaire (UMR 5803 CNRS / Université Bordeaux 1)
2001 / 2003	**Post-doctoral fellowship** / « Marie Curie Fellowship » of the European Community, University of Leiden (The Netherlands) « Quantum dynamics of multidimensional gas-surface reactions »
21 Juin 2001	**PhD in physical chemistry** / Université Bordeaux 1.
1997 / 1998	**Postgraduate diploma in Physical Chemistry** / Université Bordeaux 1
1995 / 1997	**Bachelor and Master Degrees /** Université Bordeaux 1

Languages: French, Spanish, English.

Other positions

- **Coordinator of the Master program in Physical Chemistry (PCCP)** – University of Bordeaux (since 2016)
- **Member of the Chemistry department board** – University of Bordeaux (since 2011)
- **Co-responsible for the career in physical chemistry at bachelor's degree (license)** – University of Bordeaux (since 2007)
- **Co-responsible for the career in chemistry at bachelor's degree (license)** – University of Bordeaux (since 2014)
- **Responsible of the "Theoretical and Computational Chemistry" PREFALC international program** (since 2013)
- **Local responsible of the Theoretical Chemistry French Network (RFCT)** - Université Bordeaux 1 (since 2007)
- **Head of mission in education** at the « Institut des Sciences Moléculaires – Université Bordeaux 1 » (2009-2011)
- **Head of mission in communication** for the theoretical chemistry group at the « Institut des Sciences Moléculaires – Université Bordeaux 1 » (2011-2013)

Skills

Theoretical Chemistry and computational chemistry

- Dynamics of elementary chemical reactions by means of quasi-classical methods.
- Quantum dynamics simulations (time-dependent approaches).
- Methods for multidimensional potential energy surfaces determination.
- Quantum chemistry and electronic structure calculation for periodic systems.

Teaching

Physical chemistry at bachelor's degree (license)

- General chemistry (atomic structure and spectra, chemical bond, molecular symmetry and structure, states of matter).
- Thermodynamics (first laws and concepts of thermodynamics, chemical equilibrium, kinetics of chemical reactions).
- Quantum chemistry (introduction and principles of quantum theory, atomic structure, theory of the chemical bond, molecular orbital theory, molecular modeling).
- Electronic spectroscopy.

Physical chemistry at master's degree (master) and engineering school

- Quantum chemistry (theory of the chemical bond, reactivity, molecular modeling).
- Solid state physics (electronic structure of solids, theory of phonons).

Scientific production

Publications

2017

Hot-Atoms Abstraction Dynamics of Hydrogen from Tungsten Surfaces : The Role of Surface Structure
O. Galparsoro, H.F. Busnengo, J. I. Juaristi, C. Crespos, M. Alducin, and P. Larrégaray, J. Chem. Phys. (2017), 147, 121103.

Stereodynamics of diatom formation through Eley-Rideal Abstraction
O. Galparsoro, J. I. Juaristi, C. Crespos, M. Alducin, and P. Larrégaray, J. Phys. Chem. C (2017), 121, 19849.

Classical Molecule-Surface Scattering in a Quantum Spirit: Application to H_2 / Pd(111) Non Activated Sticking
C.Crespos, J. Decock, P. Larregaray and L. Bonnet, J. Phys. Chem. C (2017), 121,16854.

2016

Hydrogen Abstraction from Metal Surfaces: When Electron-Hole Pair Excitations Strongly Affect Hot-Atom Recombination
O. Galparsoro, R. Pétuya, H.F. Busnengo, J. I. Juaristi, C. Crespos, M. Alducin, and P. Larrégaray, Phys. Chem. Chem. Phys. (2016), 18, 31378.

2015

Isotope effects in Eley-Rideal and Hot-Atom abstraction dynamics of Hydrogen from Tungsten (100) and (110) surfaces.
R. Petuya, M.A. Nosir, C. Crespos, R. Diez Muino, and P. Larregaray, J. Phys. Chem. C (2015), 119, 15325.

Energy dissipation to Tungsten surfaces upon Eley-Rideal recombination of N2 and H2.
O. Galparsoro, R. Pétuya, J. I. Juaristi, C. Crespos, M. Alducin, and P. Larrégaray, J. Phys. Chem. C (2015), 119, 15434.

Scattering of atomic Hydrogen off a H-Covered W(110) Surface : Hot-Atom versus Eley-Rideal abstraction dynamics.
R. Petuya, P. Larregaray, C. Crespos, P. Aurel, H.F. Busnengo, and A. Martinez, J. Phys. Chem. C (2015), 119, 8904.

2014

Influence of surface symmetry on the onset of Nitrogen Eley-Rideal recombination on Tungsten.
E.L. Quintas-Sanchez, P. Larregaray, C. Crespos, J. Phys. Chem. C (2014), 118, 12224.

Comparative theoretical study of H2 Eley-Rideal recombination dynamics on W(100) and W(110).
R. Pétuya, C. Crespos, E. Quintas-Sanchez, and P. Larrégaray, J. Phys. Chem. C (2014), 118, 11704.

Revisiting the nonreactive scattering of N2 off W(100) : on the influence of the scattering azimuth on in-plane angular distributions.
R. Pétuya, P.-A. Plotz, C. Crespos, and P. Larregaray, J. Phys. Chem. C (2014), 118, 21904.

2013

Surface temperature effects on the dynamics of N2 Eley-Rideal recombination on W(100).
E.L. Quintas-Sanchez, C. Crespos, P. Larrégaray, J.-C. Rayez, L. Martin-Gondre, and J. RubayoSoneira, J. Chem. Phys. (2013), 138, 024706.

2012

Dynamical reaction pathways in Eley-Rideal recombination of nitrogen from W(100).
E.L. Quintas-Sanchez, P. Larregaray, C. Crespos, L. Martin-Gondre,J. Rubayo-Soneira, J.-C. Rayez, J. Chem. Phys. (2012), 137, 064709.

Classical dynamics study of atomic oxygen over graphite (0001) with new interpolated and analytical potential energy surfaces.
V. Moron, L. Martin-Gondre, C. Crespos, P. Larregaray, P. Gamallo, R. Sayos, Comp. Theo. Chem. (2012), 990, 132.

2011

Recombination and chemical energy accommodation coefficients from chemical dynamics simulations: O/O2 mixtures reacting over a beta-cristobalite (001) surface.
V. Moron, P. Gamallo, L. Martin-Gondre, C. Crespos, P. Larregaray, R. Sayos, Phys. Chem. Chem.Phys. (2011), 13, 17494.

Seccion eficaz Eley-Rideal en la recombinación de Nitrogeno sobre Tungsteno (100).
E. Quintas-Sanchez, L. Martin-Gondre, P. Larregaray, C. Crespos, J. Rubayo-Soneira, J.-C. Rayez, Rev. Cub. Fis., (2011), 28, No. 1E, 61-65.

2010

Dinámica Eley-Rideal vs átomos-calientes en la recombinación de Nitrógeno sobre W(100).
E. Quintas-Sanchez, L. Martin-Gondre, P. Larregaray, C. Crespos, J. Rubayo-Soneira, J.-C. Rayez, Rev. Cub. Fis., (2010), 27, No. 2B, 244-250.

Dynamics simulation of N2 scattering onto W(100,110) surfaces : A stringent test for the recently developed flexible periodic London-Eyring-Polanyi-Sato potential energy surface.
L. Martin-Gondre, C. Crespos, P. Larregaray, J. C. Rayez, J. Chem. Phys. (2010), 132, 204501.

Detailed description of the flexible periodic London-Eyring-Polanyi-Sato potential energy function.
L. Martin-Gondre, C. Crespos, P. Larregaray, D. Conte, B. van Ootegem, J. C. Rayez, Chem. Phys. (2010), 367, 136.

2009

Is the LEPS potential accurate enough to investigate the dissociation of diatomic molecules on surfaces ?
L. Martin-Gondre, C. Crespos, P. Larregaray, J. C. Rayez, D. Conte and B. van Ootegem, Chem. Phys. Lett. (2009), 471, 136.

Phase-index problem in the semiclassical description of molecular collisions (correction vol 78, 062713,2008).
L. Bonnet, and C. Crespos, Phys. Rev. A (2009), 80, 059903.

2008

Phase-index problem in the semiclassical description of molecular collisions.
L. Bonnet, and C. Crespos, Phys. Rev. A (2008), 78, 062713.

DFT study of dissociative adsorption of hydrogen sulfide on Cu(111) and Au(111).
P.N. Abufager, P. G. Lustenberg, C. Crespos, and H.F. Busnengo, Langmuir (2008), 24, 14022.

2007

Modified Shepard interpolation method applied to trapping mediated adsorption dynamics (correction vol. 9, 2258, 2007).
P.N. Abufager, C. Crespos, and H.F. Busnengo, Phys. Chem. Chem. Phys. (2007), 9, 2293

Modified Shepard interpolation method applied to trapping mediated adsorption dynamics.
P.N. Abufager, C. Crespos, and H.F. Busnengo, Phys. Chem. Chem. Phys. (2007), 9, 2258

2001 - 2006

Multi-configuration time-dependent Hartree method applied to molecular dissociation on surfaces: H2 on Pt(111).
C. Crespos, H.-D. Meyer, R. Mowrey, and G.J. Kroes, J. Chem. Phys. (2006), 124, 074706.

Application of the modified Shepard interpolation method to the determination of the potential energy surface for a molecule-surface reaction.
C. Crespos, M .A. Collins, E. Pijper, and G.J. Kroes, J. Chem. Phys. (2004), 120, 2392.

Multi-dimensional potential energy surface determination by modified Shepard interpolation for a molecule-surface reaction : H2 + Pt(111).
C. Crespos, M .A. Collins, E. Pijper, and G.J. Kroes, Chem. Phys. Lett. (2003), 376, 566.

Classical dynamics of dissociative adsorption for a non activated system : role of the zero point energy.
H.F Busnengo, C. Crespos, W . Dong, A. Salin, and J.-C. Rayez, J. Chem. Phys. (2002), 116, 9005.

Role of orientational forces in non-activated molecular dissociation on a metal surface.
H.F Busnengo, C. Crespos, W . Dong, A. Salin, and J.-C. Rayez, Phys. Rev. B (2001), 63, 041402 (Rapid Communications).

Analysis of H2 dissociation dynamics on the Pd(111) surface.
C. Crespos, H .F. Busnengo, W . Dong, and A.Salin, J. Chem. Phys. (2001), 114, 10954.

Proceedings

Réactivité élémentaire gaz/solide à l'échelle moléculaire
C. Crespos, P. Larregaray, L. Martin, E.Q. Sanchez, J.C. Rayez
Proceeding 7èmés journées du Réseau Plasmas Froids, Bonascre, 29 Septembre-2 Octobre 2009.

Contribution to the microscopic description of heterogeneous chemistry at the surface of thermal protection systems of re-entry vehicles. C. Crespos, P. Larregaray, L. Martin, J.C. Rayez, E. Arquis, E. Conte, B. van Ootegem, Proceedings of the 1st international ARA days, ARA, Arcachon, 3-6 July 2006.

Improvments on catalycity determination by numerical and experimental cross checking.
B. van Ootegem, D. Conte, Ph. Tran, P. Vervisch, D. Studer, Ph. Regnier, C. Crespos, P. Larregaray, J.C. Rayez, and L. Martin, Proceeding of the 1st International ARA Days, 'Atmospheric reentry systems,missions and vehicles', Arcachon, France, July 2006.

EADS-ST approach on catalycity determination.
B. van Ootegem, D. Conte, N. Sauvage, Ph. Tran, P. Vervisch, A. Desportes, Ph. Regnier, C. Crespos, P. Larregaray, J.C. Rayez, E. Arquis and N. Perron, Proceeding of the 4th International Symposium on Atmospheric Vehicles and Systems, Arcachon, France, March 2005, AAAF.

Improvements on catalycity determination by numerical and experimental crossing.
B. van Ootegem, D. Conte,P. Tran, P. Vervisch,Ph. Regnier, C. Crespos, P. Larregaray, L. Martin, J.C. Rayez, Proceedings of the 5th European Workshop on thermal protection systems and hot structures, Noordwijk, The Netherlands, ESA SP - 631, August 2006, ISBN 92-9092-942-1.

Book chapters

Dynamics of gas-surface interactions : Atomic-level understanding of scattering processes at surfaces. Edited by R. Díez Muiño and H.F. Busnengo.
Chap. 2 : Potential Energy Surfaces for the Dynamics of Elementary Gas-Surface Processes. P. Gamallo, L. Martin-Gondre, R. Sayos, C. Crespos, P. Larregaray, ISBN 978-3-642-32955-5 – Springer Series in Surface Sciences (2013).

Multidimensional Quantum Dynamics, MCTDH theory and applications. Edited by H.-D. Meyer, F. Gatti, and G. A. Worth.
Part 3/20 Reactive and non-reactive scattering of molecules from surfaces, G. J. Kroes, R. van Harrevelt,and C. Crespos, ISBN-13 : 978-3-527 32018-9 - Wiley-VCH, Weinheim (2009).

VER/VEP Véhicules expérimentaux et d'exploration planétaire
P. Larregaray, C. Crespos, J.-C. Rayez Bordeaux 1 recherche n°6, Avril 2007, Le Pôle AESE.

Oral Communications

Revisiting dynamics of N_2 on W(100) including van der Waals interactions
A. Pena-Torres, C. Ibarguen-Becerra, H. F. Busnengo, P. Larrégaray, C. Crespos
CECAM Workshop "Challenges in reaction dynamics of gas-surface interactions and methodological advances in dissipative and non-adiabatic processes", 27-29 June 2017, Albi (France).

Dynamics of gas-surface elementary reactions: influence of van der Waals interactions
N_2/W(100)
A. Pena-Torres, C. Ibarguen-Becerra, H. F. Busnengo, P. Larrégaray, L. Bonnet, C. Crespos
Processus physico-chimiques d'interet astrophysique, 12-15 June 2017, St Florent (France).

Scattering of atomic Hydrogen off a H-Covered W(110) Surface : Hot-Atom versus Eley-Rideal abstraction dynamics
C. Crespos, R. Pétuya, P. Larrégaray, P. Aurel, H. F. Busnengo, A. E. Martínez
15th International Congress of Quantum Chemistry : Theoretical Challenges in Small Molecule Dynamics, 2-6 Juin 2015, Dalian (Chine)

Gaussian Weighting in quasi-classical trajectory method applied to molecule-surface benchmark reactions : H2+Pd ; H2+Cu
C. Crespos, J. Decock, P. Larregaray, L. Bonnet
Workshop on Atomic and Molecular Physics, 29 Juin - 3 Juillet 2015, Varadero (Cuba)

Gaussian weighting in quasi-classical trajectory method applied to molecule-surface benchmark reactions
C. Crespos, J. Decock, P. Larregaray, L. Bonnet
5th Chinese-French Workshop in Theoretical Chemistry, 10-13 Mai 2015, Strasbourg (France)

Dynamics of the Eley-Rideal Recombination of Hydrogen on Tungsten Surfaces
R. Pétuya, C. Crespos, H. F. Busnengo, A. E. Martinez, P. Larregaray
Dynamics and Reactions of hydrogen Atoms with Gold and Silver surfaces, DRAGS 3rd, 17-19 Juin 2015, Biarritz (France)

Theoretical description of the abstraction of Nitrogen and Hydrogen from Tungsten surfaces
P. Larregaray, R. Petuya, E.L. Quintas-Sanchez, C. Crespos, H.F. Busnengo, A. Martinez
Workshop on Dynamical Processes at Surfaces, 28-31 Octobre 2014, Madrid (Espagne)

Dynamique d'abstraction de l'Hydrogène de surfaces de Tungstène
P. Larregaray, R. Petuya, C. Crespos, H.F. Busnengo, A. Martinez
82e congrès de l'ACFAS, 12 au 16 Mai 2014, Montreal (Canada)

Collisions et réactivité gaz-surface : dynamique semi-classique molecule-surface
C.Crespos, P. Larregaray
Workshop Fédération de Physique Théorique et Numérique, 9-10 Janvier 2014, Bordeaux (France)

Theoretical investigation on the Eley-Rideal recombination of nitrogen on Tungsten(100)
P. Larregaray, R. Petuya, C. Crespos
Journée Scientifique du GdR Thems, 17-18 décembre 2014, Orsay (France)

Electron and Phonon excitations in diatom abstraction via Eley-Rideal mechanism from metal surfaces
O. Galparsoro-Larraza, R. Petuya, P. Larregaray, C. Crespos, M. Alducin, I. Juaristi
2eme congrès annuel du GdR ThéMS, 9-10 Décembre 2014, Talence (France)

Etude théorique de la dynamique de recombinaison de l'hydrogène sur des surfaces de tungstène
R. Pétuya, P. Larregaray, C. Crespos, H. F. Busnengo, A. E. Martinez
RCTF2014, 14eme rencontre des chimistes théoriciens francophones, 30 Juin-4 Juillet 2014, Paris (France)

Theoretical Description of the Abstraction Dynamics of Nitrogen and Hydrogen from Tungsten Surfaces
R. Petuya, C. Crespos, H. F. Busnengo, A. E. Martinez, P. Larregaray
PAMO-JSM 2014, July 7-10 2014, Reims (France)

Crystallographic anisotropy in Eley-Rideal abstraction dynamics : H+H/W(100) vs H+H/W(110)
R. Petuya, C. Crespos, P. Larregaray
5èmes Journées de Dynamique du Sud-Ouest, 4-5 Juin 2013, Perpignan (France)

Crystallographic anisotropy in Eley-Rideal abstraction dynamics : H+H/W(100) vs H+H/W(110)
R. Petuya, C. Crespos, P. Larregaray
DRAGS Meeting, 24-26 Mai 2013, HannMünden (Allemagne)

Dynamique des réactions élémentaires à l'interface gaz/solide
C. Crespos, R. Petuya, E.L. Quintas Sanchez, P. Larregaray
Processus physico-chimique d'interet astrophysique, 3-6 juin 2013, St Florent (France)

Theoretical description of H2 Eley-Rideal recombination on W(110)
R. Petuya, C. Crespos, P. Larregaray
Symposium Quantum Modeling of electronic processes in Organic Optoelectronic Devices, 7-8 novembre 2012, Bordeaux (France)

Theoretical analysis of the dynamics of N2 scattering on W(100) surface.
C. Crespos, R. Petuya, P.-A. Plotz, P. Larregaray
Workshop on Atomic and Molecular Physics, 10-14 Juillet 2012, Varadero (Cuba)

Descripción teórica de la recombinación Eley-Rideal de moléculas de nitrógeno sobre superficies de tungsteno
E. Quintas Sanchez, L. Martin, C. Crespos, P. Larregaray, L. Barrios, J. C. Rayez and J. Rubayo Soneira
Institute of Cybernetics, Mathematics and Physics (ICIMAF), 9 Novembre 2012, La Havane (Cuba)

Theoretical Analysis of N2 scattering dynamics on W(100) surface
R. Petuya, P.-A Plotz, C. Crespos, P. Larregaray
Surface Dynamics : Beyond Born Oppenheimer static surface approximation, CECAM Workshop, 24-26 Octobre 2012, Zaragoza (Espagne)

Dynamical reaction pathways in Eley-Rideal recombination of nitrogen from W(100)
E.Quintas-Sanchez, P. Larregaray, C. Crespos, L. Martin-Gondre, J.Rubayo-Soneira and J.-C. Rayez
Surface Dynamics : Beyond Born Oppenheimer static surface approximation, CECAM Workshop, 24-26 Octobre 2012, Zaragoza (Espagne)

Theoretical analysis of the molecule/surface elementary reactions
C. Crespos, P. Larregaray, L. Martin-Gondre, R. Petuya, E.L. Quintas Sanchez, J.C. Rayez
Colloque NOSSI, Nouveaux outils pour la simulation des solides et des interfaces, 6-9 Décembre 2011, Biarritz (France)
Étude théorique des mécanismes élémentaires de recombinaison de N2 sur la surface de W(100)
C. Crespos, E.L. Quintas Sanchez, P. Larrégaray, J.-C. Rayez
IVèmes Journées de Dynamique du Sud-Ouest, 7-8 Juin 2011, Pau (France)

Theoretical investigation of the Eley-Rideal recombination of Nitrogen on Tungsten(100)
C. Crespos, E.L. Quintas Sanchez, P. Larrégaray, J.-C. Rayez
ARCHES and IRSAMC workshop, 26 Mai 2011, Toulouse (France)

Theoretical investigation on the Eley-Rideal recombination of nitrogen on Tungsten(100)
E. L. Quintas Sanchez, L. Martin, P. Larregaray, C. Crespos, J.-C. Rayez, J. Rubayo-Soneira
Quinto Encuentro de Fisica y Quimica de Superficie, 27-29 Octobre 2011, Rosario (Argentine)

Theoretical investigation of the Eley-Rideal recombination of nitrogen on W(100)
E. L. Quintas Sanchez, L. Martin, P. Larregaray, C. Crespos, J.-C. Rayez, J. Rubayo-Soneira
Passion for Knowledge, 28-30 septembre 2010, San Sebastian (Espagne)

Classical reactive scattering in a semiclassical spirit
L. Bonnet, M. Gonzalez, P. Larregaray, J.-C Rayez, C. Crespos
Elementary Processes at Surfaces, Nov.30-Dec 04, 2010, Bordeaux (France)

Kinetic modeling of surface catalycity for oxygen flows over silica and carbon based surfaces from first principles
R.sayos, P. Gamallo, V. Moron, C. Crespos, P. Larregaray
Elementary Processes at Surfaces, Nov.30-Dec 04, 2010, Bordeaux (France)

Theoretical kinetic modeling of O/O2 mixtures reacting over a beta-cristobalite (100) surface
R.Sayos, P.Gamallo, V.Moron,C.Crespos, P.Larregaray
ECOSS27, 29 Aout- 3 Septembre 2010, Groningen (Pays-Bas)

Theoretical study ofoxygen dissociative adsorption on the Cu(100) surface
L.Martin-Gondre, C.Crespos„P.Larregaray, J.C.Rayez, G.Volphilac, A.Salin
ECOSS27, 29 Aout- 3 Septembre 2010, Groningen (Pays-Bas)

Theoretical kinetic modeling of O/O2 mixtures reacting over a beta-cristobalite (100) surface
R.Sayos, P.Gamallo, V.Moron,C.Crespos, P.Larregaray
Sixth International Meeting on Photodynamics, 1-5 Février 2010, La Havana (Cuba)

Réactivité élémentaire gaz/solide à l'échelle moléculaire
C. Crespos, P. Larregaray, L. Martin, E.Q. Sanchez, J.C. Rayez
7èmés journées du Réseau Plasmas Froids, Bonascre, 29 Septembre-2 Octobre 2009.

Construction de surfaces d'énergie potentielle fiables pour l'étude théorique des processus élémentaires gaz-surface.
C. Crespos, P. Larregaray, L. Martin, J.C. Rayez, D. Conte, B. van Ootegem
CiPRA3, Cinétique des Plasmas Recherche et Applications, 2-4 Avril 2008, Le Havre (France).

Dynamique des réactions élémentaires à l'interface gaz/solide
C. Crespos
Xe Journées Thématiques de Chimie Théorique, 27-28 Mars 2008, Marseille (France).

Introduction à la dynamique des réactions élémentaires gaz-surface.
C. Crespos
RFCT, Séminaires du Label National de Chimie Théorique, 29 Oct-2 Nov 2007, Bordeaux (France).

Multi-dimensional potential energy surface determination by modified Shepard interpolation for molecule-surface reactions
C. Crespos, M.A. Collins, G.J. Kroes
XXXIII QUITEL, 17-21 Septembre 2007, La Habana (Cuba)

Multi-dimensional potential energy surface determination for molecule-surface reactions
C. Crespos, M.A. Collins, G.J. Kroes
COMETXX, June 3th -7th 2007, Arcachon (France).

Dynamics of H2 dissociative adsorption on metallic surfaces
C. Crespos
Workshop GDR ARCHES, 20-23 mai 2007, Nouan le Fuzelier (France)

Construction de surfaces d'énergie potentielle multi-dimensionnelles pour la simulation de la dynamique des réactions gaz-surface : algorithme de type Shepard modifié
C. Crespos, G.J. Kroes, M.A. Collins
Journée Dynamique du Sud-Ouest, 16 Mai 2007, Toulouse (France).

Multi-dimensional potential energy surface determination by modified Shepard interpolation scheme: an application in molecule-surface reactions
C. Crespos, G.J. Kroes, M.A. Collins
6th European Conference on Computational Chemistry (EUCO-CC6), 3-7 Septembre 2006, Tale (Slovakia).

Approche théorique des phénomènes de catalycité des matériaux de protection thermique
C. Crespos, P. Larregaray, L. Martin, J.C. Rayez
Rencontre Recherche/Industrie de l'Association de Rentrée Atmosphérique, 3 Novembre 2005, Pessac (France).

Multi-dimensional potential energy surface determination for gas-surface reactions.
C. Crespos, M.A. Collins, G.J. Kroes
Comision Nacional de Energia Atomica, Centro Atomico de Bariloche, 30 Aout 2005, Bariloche (Argentine).

Kinetic modeling of surface catalycity for oxygen flows over silica and carbon based surfaces from first principles
R.sayos, P. Gamallo, V. Moron, C. Crespos, P. Larregaray.
Elementary Reactive Processes at Surfaces 2010, November 30th-December 3rd 2010, Bordeaux, France

Theoretical investigation of the Eley-Rideal recombination of nitrogen on W(100)
P. Larregaray, E. L. Quintas Sánchez, L. Martin, C. Crespos, J.-C. Rayez, J. Rubayo-Soneira
Passion for Knowledge, September 28th-September 30th, 2010, San Sebastian, Spain

Theoretical kinetic modeling of O/O2 mixtures reacting over a ß-cristobalite (100) surface
R.Sayós, P.Gamallo, V.Morón, C.Crespos, P.Larregaray
ECOSS27, August 29th-September 3rd, 2010, Groningen, The Nertherlands

Theoretical study of oxygen dissociative adsorption on the Cu(100) surface
L.Martin-Gondre, C.Crespos„ P.Larrégaray, J.C.Rayez, G.Volphilac, A.Salin
ECOSS27, August 29th-September 3rd, 2010, Groningen, The Nertherlands

Theoretical kinetic modeling of O/O2 mixtures reacting over a ß-cristobalite (100) surface
R.Sayos, P. Gamallo, V. Moron, C. Crespos, P. Larregaray
Sixth International Meeting on Photodynamics, February 1-5th 2010, Havana, Cuba

Theoretical approach of the diatomic recombination mechanisms at the gas-solid interface
E. L. Quintas Sanchez, L. Martin, P. Larregaray, C.Crespos, J.-C. Rayez. J. Rubayo Soneira
1st Workshop on Atomic and Molecular Physics,La Habana, Cuba, January 28th-30th 2009

Chemical reactions at the surface of re-entry material : a theoretical contribution
L. Martin, C. Crespos, P. Larregaray, J.C. Rayez,
Second International ARA days, October 21st-23rd, 2008, Arcachon, France

Development of a new LEPS function for the study of gas-surface reactions
L. Martin, C. Crespos, P. Larregaray, J.-C. Rayez B. van Ootegem, D. Conte
1st CTP Workshop, Elementary Gas-surface reaction from first principles, Talence, France, November 13th-14th 2008

Some theoretical contributions in heterogeneous chemistry
J.C. Rayez, L. Martin, E.L. Quintas Sanchez, C. Crespos, P. Larregaray
WATOC 2008, Sydney, September 14-19, 2008, Australia

Nouvelles Perspectives sur le traitement classique des collisions moléculaires
L. Bonnet, M.L. Gonzalez Martinez, C. Crespos, P. Larregaray, J.C. Rayez
Physique Atomique, Moleculaire et Optique, PAMO 2008, 7-10 Juillet 2008, Lille, France

Simulation classique des processus gaz-surface

P.Larregaray, C. Crespos, L.Martin, L. Bonnet, C. Diaz Blanco, A. Perrier, J.C. Rayez
Ecole du GDR Arches, 09-13 Juin 2008, Alenya, France

Développement de fonctions LEPS périodiques pour l'étude des réactions élémentaires gaz/surface.
L. Martin, C. Crespos, P. Larregaray, J.C. Rayez, E. Arquis, E. Conte, B. van Ootegem
Journées de Dynamique du Sud-Ouest, 20-21 Mai 2008, Montpellier, France.

Contribution to the microscopic description of heterogeneous chemistry at the surface of thermal protection systems of re-entry vehicles
L. Martin, C. Crespos, P. Larregaray, J.C. Rayez, E. Arquis, E. Conte, B. van Ootegem
1st international ARA days, Arcachon 3-6 July 2006, France

Improvements on catalycity determination by numerical and experimental cross checking
B. Van Ootegem, D. Conte, J. Couzi, P. Vervisch, P. Regnier, D. Studer, C. Crespos, P. Larregaray, J.-C. Rayez
5th European workshop on thermal protection systems and hot structures, Noordwijk , May 17-19, 2006, The Netherlands

Approche microphysique des phénomènes de catalycité
L. Martin, C.Crespos, P.Larrégaray, J.C. Rayez, D. Conte, B. Van Ootegem
Rencontre recherche/industrie de l'Association de Rentrée Atmosphérique, 26 Avril 2006, Talence, France

Approche théorique des phénomènes de catalycité des matériaux pour application de protection thermique
C.Crespos, P.Larrégaray, L. Martin, J.C. Rayez
Rencontre recherche/industrie de l'Association de rentrée Atmosphérique, 3 Novembre 2005, Pessac, France