Rocco Martinazzo

Università degli Studi di Milano - UMIL

Current Position

2015-present **Associate Professor**, *Faculty of Mathematical, Physical and Natural Sciences*, Dept. of Chemistry, Università degli Studi di Milano.
Italy

Previous Positions

2012-2014 **Assistant Professor**, *Faculty of Mathematical, Physical and Natural Sciences*, Dept. of Chemistry, Università degli Studi di Milano.
Italy

2004-2012 **Assistant Professor**, *Faculty of Mathematical, Physical and Natural Sciences*, Dept. of Physical Chemistry and Electrochemistry, Università degli Studi di Milano.
Italy

Education

1999–2002 **Ph.D.**, *Università degli Studi di Milano*, Milano.
Thesis title: The LiH_2^+ system: interaction forces and quantum dynamics

1992-1998 **M.Sc.**, *Università degli Studi di Milano*, Milano, *110/100 cum laude*.
Thesis title: Application of the Spin-Coupled Valence-Bond theory to the calculation of astrophysically relevant ion-molecule interaction potentials

1987-1992 **Diploma**, *ITIS Maria Curie*, Milano, *60/60*.
Technical High School for Food Technologies

Languages

Italian Mother tongue
English Fluent

Computer skills

OS Linux/Unix, MacOS, Windows
Job related Linux SA
programming Fortran, bash
typography LaTeX, Microsoft Office

Fellowships, Fundings and Awards

2018 **NEQRate**, *computational grant at CINECA HPC center, ca.* 60,000 € worth.
2017 **ASN**, *National academic qualification as Full Professor*, 03/A2, Physical Chemistry.

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2017 **ExGas**, *Grant from UMIL, Development Plan for Athenaeum*, 7,400 € worth.

2016 **EuroPAH**, *PI of the local UMIL unit acting as Partner organization of the H2020-MSCA-ITN-2016 network*, EU Grant n. 722346.

2014 **ASN**, *National academic qualification as Associate Professor*, 03/A2, Physical Chemistry.

2014 **LISA-MoIrGr**, *computational grant at CINECA HPC center*, *ca.* 80,000 € worth.

2013 **NEXT**, *Mobility grant*, Laboratoire Collisions Agrégats Réactivité, Université Paul Sabatier, Tolouse.
France

2014 **LISA-IrGraphe**, *computational grant at CINECA HPC center*, *ca.* 62,000 € worth.

2009-2011 **PRIN-2009C28YBF**, *member of the Milano research unit*.

2002-2004 **Postdoc fellow**, *Faculty of Mathematical, Physical and Natural Sciences*, Dept. of Physical Chemistry and Electrochemistry, Università degli Studi di Milano.
Italy

2004-2006 **PRIN-2004034838**, *member of the Milano research unit*.

2001-2002 **Max Planck Society**, *financial support to the visit at the Theoretical Chemistry group of prof. F. A. Gianturco*, Dept. of Chemistry, Università La Sapienza, Rome.
Italy

1992-1998 **Scholarship**, *from Istituto per il diritto allo Studio Universitario*.

1992 **Silver Medal**, *XXIVth International Chemistry Olympyads*, Pittsburg.
United States

1992 **Attestato di Benemerenza**, *for merits from the Associazione Periti Industriali di Milano*, Milano.
Italy

Experience

Research

July 2019 **WIS**, *E. Pollak*, Weizmann Institute of Science, Rehovot, Israel.
Invited scientist

2015-present **Chemical Dynamics Theory Group**, *R. Martinazzo*, Università degli Studi di Milano, Milano, Italy.
Group Leader

Spring 2013 **LCAR**, *D. Lemoine*, Université Paul Sabatier, Toulouse, France.
Invited scientist

2002-2014 **Chemical Dynamics Theory Group**, *G.F. Tantardini*, Università degli Studi di Milano, Milano, Italy.
Senior member

Winter 2005-2006 **Theoretical Chemistry Group**, *P. Saalfrank*, Institute of Chemistry, University of Potsdam, Potsdam, Germany.
Visiting scientist

2000-2002 **Theoretical Chemistry Group**, *F. A. Gianturco*, Università di Roma La Sapienza, Roma, Italy.
Visiting student

Organization of Scientific Meetings

Aug 2020 **ECOSS 35**, *35th European Conference on Surface Science*, Luxembourg, Luxembourg, Program Committee.

Apr 2020 **Challenges in reaction dynamics of gas-surface interactions**, *Methodological advances in dissipative and non-adiabatic process*, TBA, France, Co-organizer.

Aug 2018 **ECOSS 34**, *34th European Conference on Surface Science*, Aarhus, Denmark, Program Committee.

Jun 2017 **Challenges in reaction dynamics of gas-surface interactions**, *Methodological advances in dissipative and non-adiabatic process*, Albi, France, Co-organizer.

Sept 2010 **XXXIX congresso nazionale di chimica fisica**, *Organizing commitee*, Stresa, Italy.

Conferences and Workshops

June 2020 **Cosmicpah**, *Life Cycle of Cosmic PAHs*, Aarhus, Denmark, Invited Talk: TBA.

July 2019 **EPFL school**, *Advanced Electronic Structure Methods in Condensed Matter Physics*, Lausanne, Switzerland, Invited Lecture: "Quantum dyanmics in condensed phase".

March 2019 **EPoLM-4**, *4th Workshop on Energetic processing of large molecules*, Madrid, Spain, Invited Talk: "The interaction of H atoms with coronene: a quantum chemist's perspective".

Sept 2018 **ETSF**, *23rd Workshop on electronic excitations: interdisciplinary views on quantum many-body theory*, Milano, Italy, Invited Talk: "Why Silicon is not Carbon?".

Jul 2015 **13th International workshop on Quantum Reactive Scattering**, Salamanca, Spain, Invited Talk: "Quantum dynamics of hydrogen atoms on graphene".

Oct 2014 **16th Workshop on Dynamical Phenomena at Surfaces**, Madrid, Spain, Invited Talk: "Adsorption, clustering and reactions of hydrogen atoms on graphene".

May 2014 **Quantum and Classical Complexity: From Atoms to Biosystems**, Frankfurt, Germany, Invited Talk: "Effective mode representation of structured environments: towards *first principles* quantum dynamics of hydrogen atoms on graphene".

Nov 2013 **Scattering of atoms and molecules from surfaces**, Potsdam, Germany, Invited Talk: "Hydrogen atoms on graphene: structure, energetics and dynamics".

Apr 2013 **Exploring mechanisms for H_2 formation on very small carbonaceous grains and PAHs of astrophysical interest**, Toulouse, France, Invited Talk: "Adsorption and reaction of hydrogen atoms on graphitic substrates".

Apr 2013 **Rome School on Open Systems and the Quantum-Classical Boundary**, Rome, Italy, Invited Talk: "Effective mode representation of structured environments".

Sept 2012 **GrapHEL**, Mykonos, Greece, Talk: "Spin-coupling around a carbon atom vacancy in graphene".

Nov 2011 **Leiden Universiteit**, Leiden, The Netherlans, Van Marum Colluquim: "Effective mode representation of quantum mechanical energy transfer to surfaces".

Sept 2011 **Meeting ARCHES- Adsorption, Reactivite et Controle de l'Hydrogene En interaction avec des Surfaces**, Alenya, Perpignan, France, Invited Talk: "Interaction of hydrogen atoms with carbon sp^2 structures".

Sept 2011 **Challenges in modelling the reaction chemistry of interstellar dust**, Leiden, The Netherlands, Talk: "Interaction of hydrogen atoms with carbon sp^2 structures: adsorption energetics and Eley-Rideal dynamics".

May 2011 **Theoretical Molecular Dynamics with Surfaces and PAHs**, Toulose, France, Invited Talk: "Hydrogen formation on graphitic surfaces: energetics and dynamics of elementary processes".

May 2011 **GraphITA**, Gran Sasso National Laboratories, Assergi, L'Aquila, Italy, Invited Talk: "The effect of atomic-scale effects on graphene electronic structure".

Dec 2010 **Elementary Reactive Processes at Surfaces**, Bordeaux, France, Invited Talk: "Adsorption, clustering and reactions of H atoms on graphene".

Sept 2010 **ECOSS 27**, *27th European Conference on Surface Science*, Groningen, The Netherlands, Talk: "Symmetry-induced band-gap opening in graphene superlattices".

Sept 2009 **ECOSS 26**, *26th European Conference on Surface Science*, Parma, Italy, Chairman at the session: "Nanoelectronic materials and graphene".

Dec 2008 **Winter modeling workshop**, Pisa, Italy, Invited Talk: "Wavepacket approaches to system-bath quantum dynamics".

Sept 2008 **Multidimensional Quantum Mechanics with Trajectories**, *workshop organized by CCP6*, Leeds, United Kingdom, Invited Talk: "Local coherent-state approximation to system-bath quantum dynamics".

Jul 2008 **ECOSS 25**, *25 th European Conference on Surface Science*, Liverpool, United Kingdom, Invited Talk: "Theoretical study of hydrogen adsorption and dynamics on graphitic surfaces".

Feb 2008 **XXXVII Congresso Nazionale di Chimica Fisica**, Camogli (GE), Italy, Talk: "The influence of quantum reection on the Eley-Rideal hydrogen formation reaction at interstellar cloud conditions".

Aug 2007 **Elementary Reactive Processes at Surfaces**, *workshop organized by Donostia International Physics Center*, Donostia (S. Sebastian), Spain, Invited Talk:"Quantum studies of Hydrogen dynamics on graphite surfaces".

Jul 2007 **Mathematical challenges in Quantum Chemistry Problems**, *interdisciplinary workshop at the Mathematics Institute of University of Warwick*, Coventry, United Kingdom, Invited Talk: "The Local Coherent-State Approach to System-Bath Quantum Dynamics and Its Extensions".

June 2007 **The Quantum World in Real Time: Is it accessible?**, *workshop organized by the Weizmann Institute of Science*, Safed, Israel, Invited Talk: "The Local Coherent State Approach to System-Bath Quantum Dynamics".

Supervision of Graduate and Postdoctoral Fellows

2006-present **B.Sc. & M.Sc.**, $\sim$ *30 students*, Faculty of Mathematical, Physical and Natural Sciences, Dept. of Chemistry, Università degli Studi di Milano.
Italy

2006-present **Ph.D.**, *8 students*, Faculty of Mathematical, Physical and Natural Sciences, Dept. of Chemistry, Università degli Studi di Milano.
Italy

2006-present **Postdocs**, *3 fellows*, Faculty of Mathematical, Physical and Natural Sciences, Dept. of Chemistry, Università degli Studi di Milano.
Italy

Teaching

2016-present **Physical Chemistry B - Solid state**, *Master Degree in Chemistry*, Lecturer.

2016 **Mathematical methods in chemistry**, *Master Degree in Chemistry*, Lecturer.

2015-present **Physical Chemistry III**, *Bachelor Degree in Chemistry*, Lecturer.

2009-2014 **Quantum Chemistry**, *Bachelor Degree in Chemistry*, Lecturer.

2011 ***The role of phonons* in *Dynamics of molecule-surface reactions***, *Master Degree in Chemistry*, Leiden, The Netherlands, Invited lecturer.

2006-present **Theoretical Chemistry**, *Master Degree in Chemistry*, Lecturer.

2008-2010 **Quantum Chemistry**, *Bachelor Degree in Chemistry*, Lecturer.

2011,2007,2005 **Chemical Dynamics**, *a course for the Doctorate School in Chemical Sciences*, Lecturer.

2008-2010 **Physical Chemistry B (Solid State)**, *Master Degree in Chemistry*, Teaching assistant.

2004-2006 **Theoretical Chemistry**, *Master Degree in Chemistry*, Teaching assistant.

Institutional Responsibilities

2018-present **Science committee**, *Member*, Dept. of Chemistry, Università degli Studi di Milano.

2016-2019 **Chemistry Library**, *Scientific Director*, Faculty of Mathematical, Physical and Natural Sciences, Università degli Studi di Milano.

2015-2019 **HPC CINECA**, *Referent for Athenaeum*, Università degli Studi di Milano.

2015-present **Admission tests**, *Referent for Chemistry Courses*, Università degli Studi di Milano.

Memberships

2014-present **SmartMATLab**, *Smart Material Laboratory*, Unviersità degli Studi di Milano, Milano. Italy

2010-present **ISTM**, *Institute of Molecular Science and Technologies*, Consiglio Nazionale Ricerche, Roma. Italy

Evaluation Committees

2020 **Evaluator**, *Master Thesis*, Institute of Physical and Theoretical Chemistry, Goethe University of Frankfurt, Frankfurt, Germany.

2019 **Evaluator**, *Ph.D. Thesis*, Dept. of Physics, University of Milano, Milano, Italy.

2019 **Evaluation panel**, *Tenure Professorship*, Dept. of Chemistry, Università degli Studi di Milano, Milano, Italy.

2019 **Evaluator**, *Ph.D. Thesis*, Institute of Physical and Theoretical Chemistry, Goethe University of Frankfurt, Frankfurt, Germany.

2018 **Evaluation panel**, *Tenure Professorship*, Dept. of Chemistry, Università degli Studi di Milano, Milano, Italy.

2018 **Selection board**, *Assistant Professorship*, Dept. of Chemistry, Università di Sassari, Sassari, Italy.

2018 **Evaluator**, *Ph.D. Thesis*, Dept. of Chemistry, University of Barcelona, Barcelona, Spain.

2017 **Evaluator**, *Ph.D. Thesis*, Dept. of Material Chemistry and Chemical Engineering, Politecnico di Milano, Milano, Italy.

2014 **Evaluator**, *Master Thesis*, Institute of Physical and Theoretical Chemistry, Goethe University of Frankfurt, Frankfurt, Germany.

2008 **Evaluator**, *Ph.D. Thesis*, Dept. of Chemistry, Università La Sapienza, Roma, Italy.

Reviewing activity

Journals
overall > 100
(>**10**)

ACS Appl. Mater. Interfaces | ACS Nano | Carbon | Catalysis Today | Chem. Phys. Chem. Phys. Lett . | Chirality | Comp. Mat. Sci. | Int. J. Quantum Chem. | J. Comp. Phys. J. Mat. Chem. | J. Nanoparticle Res. | J. Photochem. Photobio. A |J. Phys. B: Cond. Matter J. Phys. Cond D: App. Phys. | J. Phys. Chem. A | J. Phys. Chem. C | J. Phys. Chem. Lett. **J. Chem. Phys.** | 2D Materials | Materials | Mater. Res. Express | Nanotechnology Nat. Comm. | Phys. A | Phys. B | **Phys. Chem. Chem. Phys.** | **Phys. Rev. B** **Phys. Rev. Lett.** | Phys. Rev. App. | Phys. Rev. Mat. | Phys. Scr. | Phys. Status Solidi RSC Advances | Eur. Phys. J.

Organizations
overall > 10
(>**1**)

ANR (France), **RGC** (Hong-Kong), FMO (The Netherlands), NWO (The Netherlands), ACS Petroleum Research Fund (U.S.), FWF (Austria), CINECA (Italy)
COST Association, external expert

Scientific Interests

Dissipative quantum dynamics and transport at the nanoscale
Graphene and related carbon-based materials
Real-time quantum dynamics in large systems
Interstellar chemistry

Major collaborations

Irene Burghardt	Quantum dynamics Institute of Chemistry, Goethe University of Frankfurt, Germany
Liv Hornekær	Interstellar chemistry Dept. of Physics and Astronomy, Aarhus Universitet, Denmark
Eli Pollak	Quantum mechanics Dept. of Chemical Physics, Weizmann Institute of Science, Israel
Xander Tielens	Interstellar Chemistry Leiden Observatory, Leiden Universiteit, The Netherlands

Research Impact

Source	h-index	publications	citations
ISI	24	70	1728
Scopus	24	81	1782
Google Scholar	27	NA	2532

Publication list

84 **2020**, *D. Campisi, F.D.S. Simonsen, J.D. Thrower, R. Jaganathan, L. Hornekær, R. Martinazzo and A.G.G.M. Tielens, "Superhydrogenation of pentacene: the reactivity of zigzag-edges", Physical Chemistry Chemical Physics, 22 (2020) 1557.*

83 **2019**, *A. Tripodi, D. Ripamonti, R. Martinazzo, F. Folco, T. Tabanelli, F. Cavani and I. Rossetti, "Kinetic model for the ammoxidation of ethanol to acetonitrile", Chemical Engineering Science, 207 (2019) 862.*

82 **2019**, *M. Pizzochero, M. Bonfanti and R. Martinazzo, "To Bend or Not to Bend, the Dilemma of Multiple Bonds", Physical Chemistry Chemical Physics, 22 (2019) 26342*, 2019 HOT PCCP Article.

81 **2019**, *W. Popp, M. Polkehn, K.H. Hughes, R. Martinazzo and I. Burghardt, "Vibronic coupling models for donor-acceptor aggregates using an effective-mode scheme: Application to mixed Frenkel and charge-transfer excitons in oligothiophene aggregates", Journal of Chemical Physics, 150 (2019) 244114.*

80 **2019**, *P.A. Jensen, M. Leccese, F.D.S. Simonsen, A.W. Skov, M. Bonfanti, J.D. Thrower, R. Martinazzo and L. Hornekaer, "Identification of Stable Configurations in the Superhydrogenation Sequence of Polycyclic Aromatic Hydrocarbon Molecules", Monthly Notices of the Royal Astronomical Society, 486 (2019) 5492.*

79 **2019**, *D. Lizzit, M.I. Trioni, L. Bignardi, P. Lacovig, S. Lizzit, R. Martinazzo and R. Larciprete, "Dual-Route Hydrogenation of the Graphene/Ni Interface", ACSNano, 13 (2019) 1828.*

78 **2018**, *T. Ma, M. Bonfanti, P. Eisenbrandt, R. Martinazzo, and I. Burghardt, "Multi-configurational Ehrenfest simulations of ultrafast nonadiabatic dynamics in a charge-transfer complex", The Journal of Chemical Physics, 149 (2018) 244107* .

77 **2018**, *M. Bragato, S. Achilli, F. Cragnoni, D. Ceresoli, R. Martinazzo, R. Soave and M. I. Trioni, "Magnetic Moments and Electron Transport through Chromium-Based Antiferromagnetic Nanojunctions", Materials, 11 (2018) 2030* .

76 **2018**, *M. Bonfanti and S. Achilli and R. Martinazzo, "Sticking of atomic hydrogen on graphene", Journal of Physics: Condensed Matter, 30 (2018) 283002* .

75 **2018**, *M. Bonfanti and R. Martinazzo, "Comment on 'Theoretical study of the dynamics of atomic hydrogen adsorbed on graphene multilayers' ", Physical Review B, 977 (2018) 117401* .

74 **2018**, *M. Pasquini, M. Bonfanti and R. Martinazzo, "Full quantum dynamical investigation of the Eley-Rideal reaction forming H_2 on a movable graphitic substrate at T=0 K", Physical Chemistry Chemical Physics, 20 (2018) 9779*.

73 **2017**, *E. Quartapelle Procopio, T. Benincori, G. Appoloni, P.R. Mussini, S. Arnaboldi, C. Carbonera, R. Cirilli, A. Cominetti, L. Longo, R. Martinazzo, M. Panigati and R. Po', "A family of solution-processable macrocyclic and open-chain oligothiophenes with atropoisomeric scaffolds: Structural and electronic features for potential energy applications", New Journal of Chemistry, 41 (2017), 10009*.

72 **2017**, *A. Tripodi, M. Compagnoni, R. Martinazzo, G. Ramis and I. Rossetti, "Process Simulation for the Design and Scale Up of Heterogeneous Catalytic Process: Kinetic Modelling Issues", Catalysts, 7 (2017), 159*.

71 **2016**, *F. Gottwald, M. Bonfanti, R. Martinazzo, S.D. Ivanov and O. Kuhn, "Caldeira-Leggett model describes dynamics of hydrogen atoms on graphene", Journal of Chemical Physics, 145 (2016) 126101*.

70 **2016**, *M. Bonfanti and R. Martinazzo, "Unitary Approaches to Dissipative Quantum Dynamics", in Recent Advances in Quantum Dynamics, Ed. P. Bracken (2016), InTech116*.

69 **2016**, *M. Bonfanti and R. Martinazzo, "Classical and quantum dynamics at surfaces: Basic concepts from simple models", International Journal of Quantum Chemistry, 116 (2016) 1575*, Tutorial Review, Cover Article.

68 **2016**, *T. Benincori, P.R. Mussini, R. Martinazzo, S. Arnaboldi, M. Panigati, E. Quartapelle Procopio, V. Marino, S. Casolo, F. Sannicolo', G. Appoloni, R. Cirilli, A. Pietrzyk-Le, K. Bartold, Z. Iskierko, W. Kutner and K. Noworyta, "Inherently chiral spider-like oligothiophenes", Chemistry, 22 (2016) 10839*, Cover Article.

67 **2016**, *R. Martinazzo, "Atomic-scale defects and impurities in graphene", Graphene Science Handbook - Vol. 2 Nanostructure and Atomic Arrangement, Ed.s M. Aliofkhazraei, N. Ali, W. I. Milne, C. S. Ozkan, S. Mitura, J. L. Gervasoni, CRC Press (2016)*.

66 **2016**, *M. Pizzochero, M. Bonfanti and R. Martinazzo, "Hydrogen on silicene: like or unlike graphene?", Physical Chemistry Chemical Physics, 18 (2016) 15654*.

65 **2016**, *S. Casolo, G.F. Tantardini and R. Martinazzo, "Hydrogen recombination and dimer formation on graphite from ab initio molecular dynamics simulations", Journal of Physical Chemistry A, 120 (2016) 5032*.

64 **2016**, *G. L. Chiarello, A. Zuliani, D. Ceresoli, R. Martinazzo and E. Selli, "Exploiting the photonic crystal properties of TiO_2 nanotube arrays to enhance photocatalytic hydrogen production", ACS Catalysis, 6 (2016) 1345*.

63 **2016**, *M. Pasquini, M. Bonfanti and R. Martinazzo, "Quantum dynamical investigation of the isotope effect in H_2 formation on graphite at cold collision energies", Physical Chemistry Chemical Physics, 18 (2016) 6607*.

62 **2015**, *M. Bonfanti, B. Jackson, K. H. Hughes, I. Burghardt and R. Martinazzo, "Quantum dynamics of hydrogen atoms on graphene: II Sticking", Journal of Chemical Physics, 124 (2015) 124704.*

61 **2015**, *M. Bonfanti, B. Jackson, K. H. Hughes, I. Burghardt and R. Martinazzo, "Quantum dynamics of hydrogen atoms on graphene: I System-bath modeling", Journal of Chemical Physics, 124 (2015) 124703.*

60 **2015**, *M. Pizzochero, O. Leenaerts, B. Partoens, R. Martinazzo and F. Peeters, "Hydrogen adsorption on boron and nitrogen doped graphene", Journal of Physics: Condensed Matter, 27 (2015) 425502.*

59 **2015**, *M. Bonfanti, K. H. Hughes, I. Burghardt and R. Martinazzo, "Vibrational relaxation and decoherence in structured environments: a numerical investigation", Annalen der Physik, in press, http://dx.doi.org/10.1002/andp.201500144.*

58 **2015**, *P .Bonardi, S. Achilli, G. F. Tantardini and R. Martinazzo, "Electron transport in carbon wires contacted to Ag electrodes: a detailed* first principles *investigation", Physical Chemistry Chemical Physics, 17 (2015) 18413.*

57 **2014**, *F. Sannicolo, P.R. Mussini, T. Benicori, R. Cirilli, S. Abbate, S. Arnaboldi, S. Casolo, E. Castiglioni, G. Longhi, R. Martinazzo, M. Panigati, M. Pappini, E. Quartapelle Procopio, and S. Rizzo, "Inherently Chiral Macrocyclic Oligothiophenes: Easily Accessible Electrosensitive Cavities with Outstanding Enantioselection Performances", Chemistry, 20 (2014) 15298*, Cover Article.

56 **2014**, *M. Bonfanti, G. F. Tantardini and R. Martinazzo, "Adiabatic potential energy surfaces for the low energy collisional dynamics of C^+ ions with H_2 molecules", The Journal of Physical Chemistry A, 118 (2014) 6595.*

55 **2014**, *S. Achilli, G. F. Tantardini and R. Martinazzo, "Hydrogen-dimer lines and electron waveguides in graphene", Physical Chemistry Chemical Physics, 16 (2014) 17610 .*

54 **2014**, *G. Longhi, S. Abbate, G. Mazzeo, E. Castiglioni, P. Mussini, T. Benicori, R. Martinazzo and F. Sannicolo, "Structural and Optical Properties of Inherently Chiral Polythiophenes: A Combined CD-Electrochemistry, Circularly Polarized Luminescence and TDDFT Investigation", The Journal of Physical Chemistry C, 118 (2014) 16019.*

53 **2014**, *K. H. Hughes, B. Cahier, R. Martinazzo, H. Tamura and I. Burghardt, "Non-Markovian reduced dynamics of ultrafast charge transfer at an oligothiphene-fullerene heterojunction", Chemical Physics, 442 (2014) 111 .*

52 **2014**, *M. Caratelli, S. Casolo, G.F. Tantardini and R. Martinazzo, "Structure and stability of hydrogenated carbon atom vacancies in graphene", Carbon, 77 (2014) 165.*

51 **2013**, *M. Caratelli, S. Casolo, G.F. Tantardini and R. Martinazzo, "Spin coupling around a carbon atom vacancy in graphene", Phys. Rev. B, 88 (2013) 195424.*

50 **2013**, *S. Casolo, G.F. Tantardini and R. Martinazzo, "Insights into hydrogen formation in space from ab initio molecular dynamics", PNAS, 110 (2013) 6674 .*

49 **2013**, *R. Martinazzo, S. Casolo and L. Hornekaer, "Hydrogen recombination on graphitic surfaces", in "Dynamics of Gas-Surface Interactions", Ed.s R. D. Muino and H. F. Busnengo, Springer-Verlag (2013) .*

48 **2012**, *I. Burghardt, R. Martinazzo, and K. H. Hughes, "Non-Markovian reduced dynamics based upon a hierarchical effective-mode representation", J. Chem. Phys., 137 (2012) 144107.*

47 **2012**, *H. Tamura, R. Martinazzo, M. Ruckenbauer, and I. Burghardt, "Quantum dynamics of ultrafast charge transfer at a polymer-fullerene interface", J. Chem. Phys., 137 (2012) 22A540.*

46 **2012**, *M. Bonfanti, G. F. Tantardini, K. H. Hughes, R. Martinazzo and I. Burghardt, "Compact MCTDH wavefunctions for high-dimensional system-bath quantum dynamics", J. Phys. Chem. A, 116 (2012) 11406.*

45 **2012**, *F. Bouakhline, F. Luder, R. Martinazzo and P. Saalfrank, "Reduced and Exact Quantum Dynamics of the Vibrational Relaxation of a Molecular System Interacting with a Finite-Dimensional Bath", J. Phys. Chem. A, 116 (2012) 11118.*

44 **2012**, *R. Martinazzo, K. H. Hughes and I. Burghardt, "Hierarchical effective-mode approach for extended molecular systems", in "Advances in the Theory of Quantum Systems in Chemistry and Physics", Eds. P. Hoggan, J. Maruani, P. Piecuch, G. Delgado-Barrio, E. J. Braendas, PTCP (Progress in Theoretical Chemistry and Physics) Series, Springer Verlag (2012) vol. 22, part 5, pp-269-283.*

43 **2011**, *M. Bonfanti, S. Casolo, G.F. Tantardini, A. Ponti and R. Martinazzo, "A few simple rules governing hydrogenation of graphene dots", J. Chem. Phys., 135 (2011) 164701.*

42 **2011**, *R. Martinazzo, K. H. Hughes, and I. Burghardt, "Unravaling a Brownian particle's memory with effective mode chains", Phys. Rev. E (Rapid Communication), 84 (2011) 030102(R).*

41 **2011**, *M. Bonfanti, S. Casolo, G.F. Tantardini and R. Martinazzo, "Surface models and reaction barrier in Eley-Rideal formation of H_2 on graphitic surfaces", Phys. Chem. Chem. Phys., 13 (2011) 16680.*

40 **2011**, *F. Sterpone, R. Martinazzo, A. N. Panda, I. Burghardt, "Coherent excitation transfer driven by torsional dynamics: a model Hamiltonian for PPV type systems", Z. Phys. Chem., 225 (2011) 441.*

39 **2011**, *S. Lopez-Lopez, R. Martinazzo and M. Nest, "Benchmark calculations for dissipative dynamics of a system coupled to an anharmonic bath with the Multi-Configuration Time-Dependent Hartree method", J. Chem. Phys., 134 (2011) 094102.*

38 **2011**, *S. Casolo, R. Martinazzo and G.F. Tantardini, "Band Engineering in Graphene with Superlattices of Substitutional Defects", J. Phys. Chem. C, 115 (2011) 3250 (first version on arXiv, http://arxiv.org/abs/1008.4706).*

37 **2011**, *R. Martinazzo, B. Vacchini, K. H. Hughes, and I. Burghardt, "Universal Markovian reduction of Brownian particle dynamics", J. Chem. Phys. (Communication), 134 (2011) 011101.*

36 **2011**, *S. Lopez-Lopez, M. Nest and R. Martinazzo, "Generalized CC-TDSCF and LCSA: the system energy representation", J. Chem. Phys., 134 (2011) 014102.*

35 **2011**, *I. Burghardt, K. H. Hughes, R. Martinazzo, H. Tamura, E. Gindensperger, H. Koeppel, L. S. Cederbaum, "Conical intersections coupled to an environment", in: "Conical Intersections: Theory, Computation, and Experiment", Advanced Series in Physical Chemistry, vol. 17, W. Domcke, D. R. Yarkony, H. Koeppel (Eds.), World Scientific, Singapore, 301-346, 2011.*

34 **2011**, *R. Martinazzo, S. Casolo, G.F. Tantardini, "The effect of atomic-scale defects and dopants on the electronic structure of graphene", in "Physics and applications of Graphene - Theory", Ed. S. Mikhailov, Intech, 2011.*

33 **2010**, *R. Martinazzo, K. H. Hughes, F. Martelli, and I. Burghardt, "Effective spectral densities for system-environment dynamics at conical intersections: S2-S1 conical intersection in pyrazine", Chem. Phys., 377 (2010) 21 (H. Koeppel Festschrift).*

32 **2010**, *R. Martinazzo, S. Casolo, G.F. Tantardini, "Symmetry-induced band-gap opening in graphene superlattices", Physical Review B 81 (2010) 245420, (first version on arXiv:0910.2407v1, 2009).*

31 **2009**, *S. Casolo, R. Martinazzo, M. Bonfanti and G. F. Tantardini, "Quantum Dynamics of the Eley-Rideal Hydrogen Formation Reaction on Graphite at Typical Interstellar Cloud Conditions", Journal of Physical Chemistry A, 113 (2009) 14545.*

30 **2009**, *S. Casolo, O. M. Lovvik, R. Martinazzo and G. F. Tantardini, "Understanding adsorption of hydrogen atoms on graphene", Journal of Chemical Physiscs 130 (2009) 054704 (first version on arXiv:0808.1312v1, 2008).*

29 **2008**, *R. Martinazzo, I. Burghardt, F. Martelli and M. Nest, "Local coherent-state approximation to system-bath quantum dynamics", in Multidimensional Quantum Mechanics with Trajectories, Eds: D. Shalashilin, M. P. de Miranda, CCP6, 2008, ISBN 978-0-9545289-8-0.*

28 **2008**, *I. Burghardt, R. Martinazzo, F. Martelli and G. Worth, "The G-MCTDH method: related system-bath dynamics using Gaussian wavepackets", in Multidimensional Quantum Mechanics with Trajectories, Eds: D. Shalashilin, M. P. de Miranda, CCP6, 2009, ISBN 978-0-9545289-8-0.*

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