# Rocco Martinazzo

Università degli Studi di Milano - UMIL

## Current Position

2023-present **Full Professor of Physical Chemistry** , *Faculty of Mathematical, Physical and Natural Sciences*, Dept. of Chemistry, Università degli Studi di Milano.
Italy

## Previous Positions

2015-2023 **Associate Professor**, *Faculty of Mathematical, Physical and Natural Sciences*, Dept. of Chemistry, Università degli Studi di Milano.
Italy

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 | programming | Fortran, bash, Python |
| Job related | Linux SA | typography | LaTeX, Microsoft Office |

*v. Golgi 19, Milano – 20133 – Italy*
*+39 0250314287* • *+39 0250314300* • *rocco.martinazzo@unimi.it*
*users.unimi.it/cdtg*

## 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.

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 2022 **ECOSS 35**, *35th European Conference on Surface Science*, Luxembourg, Program Committee..

Sept 2021 **Challenges in reaction dynamics of gas-surface interactions**, *Methodological advances in dissipative and non-adiabatic process*, Toulouse, 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

Dec 2022 **TCP**, *Theoretical Chemical Physics Workshop*, Luxembourg, Luxemborug, Invited talk: "Quantum theory of electronic friction".

Sept 2022 **CHAMPS**, *Exact factorization and Bohmian Mechanics*, Bristol, United Kingdom, Invited talk: "Quantum theory of electronic friction".

Jun 2022 **Marvel**, *First-Principles modelling of Defects in Solids*, ETH Zurich, Switzerland, Invited talk: "Atomic-scale defects in graphene".

Feb 2022 **DQML**, *Dynamics, Quantum Effects and Machine Learning in Materials Science and Computational Chemistry*, Hintertux, Austria, Invited talk: "Quantum dynamics in condensed phases".

June 2021 **Marvel**, *First-Principles modelling of Defects in Solids*, ETH Zurich, Switzerland, Invited Talk: TBA.
Postponed to 2022 due to Covid-19

June 2020 **Cosmicpah**, *Life Cycle of Cosmic PAHs*, Aarhus, Denmark, Invited Talk: TBA.
Postponed to 2022 due to Covid-19

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".

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".

## Invited Seminars

Apr 2023 **Cambridge**, *Department of Chemistry*, Cambridge, United Kingdom, "Quantum theory of electronic friction" .

Oct 2022 **InterCat**, *Center for Interstellar Catalysis*, Aarhus, Denmark , "Hydrogen adsorption and reaction on sp2 carbon structures: energetics and dynamics" (webinar).

Jul 2021 **CINN**, *Catalan Institute of Nanoscience and Nanotechnology*, Stephen Roche's group, Barcelona, Spain, "Graphene as a quantum pinball" (Webinar).

Feb 2015 **GIF**, *Goethe-Universität Frankfurt am Main*, Irene Burghardt's group, Frankfurt, Germany, "Quantum dynamics of hydrogen atoms on graphene".

Apr 2013 **UPS-LCAR**, *Université Paul Sabatier*, Christine Joblin's group, Toulouse, France, "Interaction of hydrogen atoms with sp2 carbon atoms".

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

Jun 2011 **AU**, *Aarhus University*, Liv Hornekaer's group, Aarhus, Denmark, "Hydrogen formation on graphitic surfaces: energetics and dynamics of elementary processes".

Feb 2011 **TUM**, *Technische Universität München*, Mathias Nest's group, Munich, Germany, "Generalized LCSA dynamics: the energy representation".

Dec 2010 **UP**, *Universität Potsdam*, Peter Saalfrank's group, Potsdam, Germany, "Reaction of H atoms on graphene".

Nov 2009 **UDE**, *Universität Duisburg-Essen*, Eckart Hasselbrink – Peter Kratzer groups, Duisburg, Germany, "Tailoring graphene electronic properties via adsorption of hydrogen atoms".

Jun 2009 **UT**, *Universität Tübingen*, Christian Lubich's group, Tübingen, Germany, "Wavepacket approaches to system-bath quantum dynamics".

Dec 2008 **UP**, *Universität Potsdam*, Peter Saalfrank's group, Potsdam, Germany, "Understanding adsorption of hydrogen atoms on graphenic substrates".

Apr 2008 **USi**, *Università di Siena*, Carlo Petrongolo's group, Siena, Italy, "Carbon chemistry in the interstellar medium and the CH+ mystery".

Feb 2008 **UP**, *Universität Potsdam*, Peter Saalfrank's group, Potsdam, Germany, "System-bath dynamics with the Local Coherent State Approximation".

## 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.

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

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

2022-present **HPC@Unimi: INDACO for molecules and solids**, *a course for the Doctorate School in Chemical Sciences*, Lecturer.

2016-present **Literature Search in Chemistry**, *a course for the Doctorate School in Chemical Sciences*, Lecturer.

2016 **Mathematical methods in chemistry**, *Master 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.

2007,2005 **Chemistry at Surfaces**, *a course for the Doctorate School in Chemical Sciences*, Lecturer.

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

2023- **QA**, *Referent*, Dept. of Chemistry, Università degli Studi di Milano.

2020- **INDACO (HPC Unitech)**, *Chemistry referent*, Università degli Studi di Milano.

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

2020-2022 **BICF (Scientific Library)**, *Chemistry referent*, 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<br>*overall* > 100<br>(>**10**) | Acc. Chem. Res. \| ACS Appl. Mater. Interfaces \| ACS Nano \| Adv. Electron. Mater. \| Carbon \| Catalysis Today \| Chem. Phys. \| Chem. Phys. Lett . \| Chirality \| Comp. Mat. Sci.<br>Int. J. Quantum Chem. \| J. Comp. Phys. \| J. Mat. Chem. \| J. Nanoparticle Res.<br>J. Photochem. Photobio. A \|J. Phys. B: Cond. Matter \| J. Phys. Cond D: App. Phys.<br>J. Phys. Chem. A \| J. Phys. Chem. C \| J. Phys. Chem. Lett.<br>**J. Chem. Phys.** \| 2D Materials \| Materials \| Mater. Res. Express \| Nanotechnology \| Nanoletters<br>Nat. Comm. \| Phys. A \| Phys. B \| **Phys. Chem. Chem. Phys.** \| **Phys. Rev. B**<br>**Phys. Rev. Lett.** \| Phys. Rev. App. \| Phys. Rev. Mat. \| Phys. Rev. X \| Phys. Scr.<br>Phys. Status Solidi \| RSC Advances \| Eur. Phys. J. |
| Organizations<br>*overall* > 10<br>(>**1**) | **ANR** (France), **RGC** (Hong-Kong), FMO (The Netherlands), NWO (The Netherlands),<br>ACS Petroleum Research Fund (U.S.), FWF (Austria), CINECA (Italy), FARE-MIUR (Italy)<br>COST Association, external expert |

## Scientific Interests

Dissipative quantum dynamics and transport at the nanoscale

Real-time quantum dynamics in large systems

Graphene and related carbon-based materials

Interstellar chemistry

Quantum computing

Theory of chemical bond

## Major collaborations

| | |
|---|---|
| Irene Burghardt | Quantum dynamics<br>Institute of Chemistry, Goethe University of Frankfurt, Germany |
| Liv Hornekær | Interstellar chemistry<br>Dept. of Physics and Astronomy, Aarhus Universitet, Denmark |
| Eli Pollak | Quantum mechanics<br>Dept. of Chemical Physics, Weizmann Institute of Science, Israel |
| Ivano Tavernelli | Quantum computing<br>IBM research, Zurich Research Laboratory, Zurich, Switzerland |
| Xander Tielens | Interstellar Chemistry<br>Leiden Observatory, Leiden Universiteit, The Netherlands |

## Research Impact

| Source | h-index | publications | citations |
|---|---|---|---|
| ISI | 28 | 94 | 2319 |
| Scopus | 28 | 101 | 2402 |
| Google Scholar | 30 | NA | 3010 |

| | |
|---|---|
| Average Self-Citation rate (from author) | 13.2% |
| Average Self-Citation rate (from all authors) | 25.4% |

(Source: Scopus)

## Publication list

103 **2022**, *P.J. Ollitrault, S. Jandura, A. Miessen, I. Burghardt, R. Martinazzo, F. Tacchino and I. Tavernelli, "Quantum algorithms for grid-based variational time evolution", submitted.*

102 **2022**, *Y. Litman, E.S. Pós, C.L. Box, R. Martinazzo, R.J. Maurer and M. Rossi, "Dissipative Tunneling Rates through the Incorporation of First-Principles Electronic Friction in Instanton Rate Theory. II Benchmarks and applications", submitted.*

101 **2022**, *Y. Litman, E.S. Pós, C.L. Box, R. Martinazzo, R.J. Maurer and M. Rossi, "Dissipative Tunneling Rates through the Incorporation of First-Principles Electronic Friction in Instanton Rate Theory. I Theory", submitted.*

100 **2022**, *R. Martinazzo and I. Burghadt, "Quantum dynamics with electronic friction", Physical Review Letters, accepted paper.*

99 **2022**, *R. Martinazzo and I. Burghadt, "Quantum theory of electronic friction", Physical Review A, accepted paper.*

98 **2022**, *B. Blasiak, D. Brey, W. Koch, R. Martinazzo and I. Burghadt, "Modelling Ultrafast Dynamics at a Conical Intersection with Regularized Diabatic States: An Approach Based on Multiplicative Neural Networks", submitted.*

97 **2022**, *D. Brey, R. Binder, R. Martinazzo and I. Burghadt, "Signatures of coherent vibronic exciton dynamics and conformational control in two-dimensional electronic spectroscopy of conjugated polymers", Faraday Discussion, accepted paper.*

96 **2022**, *R. Ireland, P. Jeszenszki, E. Matyus, R. Martinazzo, M. Ronto and E. Pollak, "Lower bounds for non-relativistic atomic energies", ACS Physical Chemistry Au, 2 (2022) 23.*

95 **2021**, *M. Ronto, E. Pollak and R. Martinazzo, "Comparison of an Improved Self-consistent Lower Bound Theory with Lehmann's Method for Low-lying Eigenvalues", Scientific Reports, 23450 (2021) 11.*

94 **2021**, *R. Martinazzo and I. Burghardt, "Comment on 'Regularizing the MCTDH equations of motion through an optimal choice on-the-fly (i.e., spawning) of unoccupied single-particle functions'", arXiv (2021) 2102.12117.*

93 **2021**, *M. Cappelletti, M. Leccese, M. Cococcioni, D. M. Proseprio and R. Martinazzo, "The different story of $\pi$ bonds", Molecules, 26 (2021) 3805.*

92 **2021**, *E. Pollak and R. Martinazzo, "Lower bounds for Coulombic systems", Journal of Chemical Theory and Computation, 17 (2021) 1535.*

91 **2021**, *D. Campisi, T. Lamberts, N.Y. Dzade, R. Martinazzo, I.L. ten Kate, A.G.G.M. Tielens, "Interaction of Aromatic Molecules with Forsterite: Accuracy of the Periodic DFT-D4 Method", Journal of Physical Chemistry A, 125 (2021) 2770.*

90 **2020**, *A Tripodi, R. Martinazzo, G Ramis and I Rossetti, "Process Modeling Issues in the Design of a Continuous-Flow Process for the Production of Ibuprofen", Chemical Engineering & Technology 43 (2020), 2557.*

89 **2020**, *A. Bossi, S. Arnaboldi, C. Castellano, R. Martinazzo and S. Cauteruccio, "Benzodithienyl Silanes for Organic Electronics: AIE Solid-State Blue Emitters and High Triplet Energy Charge-Transport Materials", Advanced Optical Materials, 8 (2020) 2001018.*

88 **2020**, *E. Pollak and R. Martinazzo, "Self-consistent theory of lower bounds for eigenvalues", The Journal of Chemical Physics, 115 (2020) 244110.*

87 **2020**, *R. Martinazzo and E. Pollak, "Lower bounds to eigenvalues of the Schroedinger equation by solution of a 90-y challenge", Proceedings of the National Academy of Sciences of the United States of America, 117 (2020) 16181.*

86 **2020**, *R. Martinazzo and I. Burghardt, "Local-in-Time error in variational quantum dynamics", Physical Review Letters, 124 (2020) 150601.*

85 **2020**, *G. Bonetti, S. Arnaboldi, S. Grecchi, G. Appoloni, E. Massolo, S. Rossi, R. Martinazzo, F. Orsini, P. R. Mussini, T. Benincori, "Effective Enantiodiscrimination in Electroanalysis Based on a New Inherently Chiral 1,1'-binaphthyl Selector Directly Synthesizable in Enantiopure Form", Molecules, 25 (2020) 2175.*

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, 527 (2015) 556.*

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.*

27 **2008**, *I. Pino, R. Martinazzo and G. F. Tantardini, "Quasi-classical trajectory study of the adiabatic reactions occurring on the two lowest-lying electronic states of the LiH2+ system", Physical Chemistry Chemical Physics, 10 (2008) 5545.*

26 **2007**, *R. Martinazzo, I. Pino, S. Casolo and G. F. Tantardini, "Simulating chemical processes from scratch: classical and quantum molecular dynamics", CILEA report 2007.*

25 **2007**, *M. Bonfanti, R. Martinazzo, G. F. Tantardini and A. Ponti, "Physisorption and Diffusion of Hydrogen Atoms on Graphite from Correlated Calculations on the H-Coronene Model System", Journal of Physical Chemistry C, 111 (2007) 5825.*

24 **2007**, *G. Lanzani, R. Martinazzo, G. Materzanini, I. Pino and G.F. Tantardini, "Chemistry at surfaces: from ab initio structures to quantum dynamics", Theoretical Chemistry Accounts, 117 (2007) 805.*

23 **2006**, *P. Saalfrank, I. Andrianov, S. Beyvers, Y. Ohtsuki and R. Martinazzo, "System-Bath Quantum Dynamics of Vibrational Excitation and Relaxation of Adsorbates", in Dynamics of Open Quantum Systems, Eds: K. Hughes, CCP6, 2006.*

22 **2006**, *R. Martinazzo, M. Nest, P. Saalfrank and G. F. Tantardini, "A local coherent-state approximation to system-bath quantum dynamics", Journal of Chemical Physics, 125 (2006) 194102.*

21 **2006**, *R. Martinazzo and G. F. Tantardini, "Quantum study of Eley-Rideal reaction and Collision Induced Desorption of hydrogen atoms on a graphite surface: II. H-physisorbed case", Journal of Chemical Physics, 124 (2006) 124703.*

20 **2006**, *R. Martinazzo and G. F. Tantardini, "Quantum study of Eley-Rideal reaction and Collision Induced Desorption of hydrogen atoms on a graphite surface: I. H-chemisorbed case", Journal of Chemical Physics, 124 (2006) 124702.*

19 **2005**, *R. Martinazzo and G. F. Tantardini, "Quantum effects in exoergic, barrierless reaction at high collision energies", Journal of Physical Chemistry A, 109 (2005) 9379.*

18 **2005**, *R. Martinazzo and G. F. Tantardini, "Testing wavepacket dynamics in computing radiative association cross-sections", Journal of Chemical Physics, 122 (2005) 094109.*

17 **2004**, *R. Martinazzo, S. Assoni, G. Marinoni, G.F. Tantardini, "Hot-Atom vs Eley-Rideal dynamics in hydrogen recombination on Ni(100). I The single-adsorbate case", Journal of Chemical Physics, 120 (2004) 8761.*

16 **2004**, *G. Calderoni, F. Cargnoni, R. Martinazzo, and M. Raimondi, "Potential energy surface, bound states, and rotational inelastic cross sections of the He-CH4 system: A theoretical investigation", Journal of Chemical Physics, 121 (2004) 8261.*

15 **2003**, *E. Bodo, R. Martinazzo and F.A. Gianturco, "Two exothermic reactions in the Lithium Chemistry Network", in High Accuracy Potentials for Quantum Dynamics, Eds: A. Miani, J. Tennyson and T. van Mourik, 2003.*

14 **2003**, *R. Martinazzo, G.F. Tantardini, E. Bodo, F.A. Gianturco, "Accurate Potential Energy Surfaces for the study of lithium-hydrogen ionic reactions", Journal of Chemical Physics, 119 (2003) 11241.*

13 **2003**, *E. Bodo, F.A. Gianturco, R. Martinazzo, "The Gas-Phase Lithium Chemistry in the Early Universe: Elementary Processes, Interaction Forces and Quantum Dynamics", Physics Reports, 384 (2003) 85.*

12 **2003**, *R. Martinazzo, E. Bodo, F.A. Gianturco, "A modified Variable-Phase algorithm for multichannel scattering with long-range potentials", Computer Physics Communications, 151 (2003) 187.*

11 **2003**, *R. Martinazzo, E. Bodo, F.A. Gianturco, "Three-dimensional reactive surfaces for the LiH2+ system: an analysis of accurate ab -initio results", Chemical Physics, 287 (2003) 335.*

10 **2003**, *M. Satta, E. Bodo, R. Martinazzo, F.A. Gianturco, "Photoexcitation of LiH2+ from selected initial states: a time dependent model", Journal of Chemical Physics, 117 (2002) 177.*

9 **2002**, *M. Sironi, M. Raimondi, R. Martinazzo, F.A. Gianturco, D.L Cooper, "Recent developments of the SCVB method", in Theoretical and Computational Chemistry, vol.10 - Valence Bond Theory, D.L. Cooper (ed.), Elsevier Science B.V., 2002.*

8 **2001**, *E. Bodo, F.A. Gianturco, R. Martinazzo, M. Raimondi, "Reactive behaviour of the system: II. Collision Induced Dissociation and Reaction in the collinear LiH+ + H dynamics from time dependent calculations", Journal of Physical Chemistry A, 105 (2001) 10994.*

7 **2001**, *E. Bodo, F.A. Gianturco, R. Martinazzo, M. Raimondi, "Reactive behaviour of the system: I. The evaluation of the lower lying PESs for the collinear geometries", Journal of Physical Chemistry A, 105 (2001) 10986.*

6 **2001**, *E. Bodo, F.A. Gianturco, R. Martinazzo and M. Raimondi, "Computed orientational anisotropy and vibrational couplings for the LiH + H interaction potential", European Physics Journal D, 15 (2001) 321.*

5 **2001**, *E.Bodo, F.A. Gianturco, R. Martinazzo, M. Raimondi, "Possible reaction paths in the LiH2+ chemistry: a computational analysis of the interaction forces", Chemical Physics, 271 (2001) 309.*

4 **2001**, *R. Martinazzo, A. Famulari, M. Raimondi, E. Bodo, F.A. Gianturco, "A MultiReference Valence Bond approach to electronic excited states", Journal of Chemical Physics, 115 (2001) 2917.*

3 **2000**, *E. Bodo, F.A Gianturco, R. Martinazzo, A. Forni, A. Famulari, M. Raimondi, "Spatial energetics of protonated LiH: lower lying potential energy surfaces from Valence Bond calculations", Journal of Physical Chemistry A, 104 (2000) 11972.*

2 **2000**, *R. Specchio, A. Famulari, R. Martinazzo, M. Raimondi "Applications of a variational coupledelectron pair approach to the calculation of intermolecular interaction in the framework of the VB theory: Study of the He-CH4 van der Waals complex", Journal of Chemical Physics, 113 (2000), 6724.*

1 **2000**, *E. Bodo, F.A Gianturco, R. Martinazzo, F. Paesani, M. Raimondi "Testing van der Waals interactions with quantum dynamics: repulsive anisotropy and well depth in the LiH + He system", Journal of Chemical Physics, 113 (2000) 11071.*

May 24, 2023

*v. Golgi 19, Milano – 20133 – Italy*
*+39 0250314287 • +39 0250314300 • rocco.martinazzo@unimi.it*
*users.unimi.it/cdtg*