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

Fellowships, Fundings and Awards

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2024 **MALAMP**, *PI of Chemistry research unit*, PNRR ICSC, *ca.* 200,000 € worth (total).

2023 χ**ISS**, *PI of Milano research unit*, PRIN-2022 Grant no. FL4NZ4, *ca.* 200,000 € worth (total).

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, ca. 4,000,000 € worth (total).

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, ca. 8000 € worth.

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

Giu 2023 **Warwick**, *Warwick Center for Predictive Modelling*, Warwick, United Kingdom, "Quantum dynamics with a multitude of electronic states" .

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.**, ∼ *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

2024- **Dept. of Chemistry**, *Vice-Director*, Università degli Studi di Milano.

2023-2024 **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

2024 **Evaluator**, *Ph.D. Thesis*, Dept. of Physics, University of Luxembourg, Luxembourg.

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**)	Acc. Chem. Res. | ACS Appl. Mater. Interfaces | ACS Nano | Adv. Electron. Mater. | 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 | Nanoletters Nat. Comm. | Phys. A | Phys. B | **Phys. Chem. Chem. Phys.** | **Phys. Rev. B** **Phys. Rev. Lett.** | Phys. Rev. App. | Phys. Rev. Mat. | Phys. Rev. X | 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), FARE-MIUR (Italy) COST Association, external expert

Scientific Interests

Spin and chirality
Topology and geometry in chemistry and condensed matter physics
Dissipative quantum dynamics and transport at the nanoscale
Real-time quantum dynamics in large systems
Graphene and related carbon-based materials
Quantum computing
Theory of chemical bond
Interstellar chemistry

Major collaborations

Irene Burghardt	Quantum dynamics Institute of Chemistry, Goethe University of Frankfurt, Germany
Matteo Cococcioni	Spin, condensed matter physics Dept. of Physcs, Università di Pavia, Pavia
Eli Pollak	Quantum mechanics Dept. of Chemical Physics, Weizmann Institute of Science, Israel
Ivano Tavernelli	Quantum computing IBM research, Zurich Research Laboratory, Zurich, Switzerland

Research Impact

Source	h-index	publications	citations
ISI	29	102	2569
Scopus	29	111	2662
Google Scholar	33	NA	3340

Average Self-Citation rate (from author)	13.2%
Average Self-Citation rate (from all authors)	25.4%
(Source: Scopus)	

Publication list

110 **2024**, R. Martinazzo and I. Burghardt, *"Emergence of the molecular geometric phase from exact electron-nuclear dynamics", accepted in Journal of Physical Chemistry Letters.*

109 **2024**, *O. Bridge, P. Lazzaroni, R. Martinazzo, M. Rossi, S.C. Althorpe and Y. Litman, "Quantum rates in dissipative systems with spatially varying friction", Journal of Chemical Physics 161 (2024) 024110 , 243002.*

108 **2024**, *R. Martinazzo and I. Burghardt, "Dynamics of the molecular geometric phase", Physical Review Letters 132 (2024), 243002.*

107 **2023**, *R. Martinazzo and I. Burghardt, "Quantum hydrodynamics of coupled electron-nuclear systems", arXiv preprint arXiv:2310.08766.*

106 **2023**, *M. Leccese and R. Martinazzo, "Anomalous delocalization of resonant states in graphene & the vacancy magnetic moment", Electronic Structure 5 (2023), 024010.*

105 **2023**, *M. Leccese, R. Jaganathan, L. Slumstrup, J.D. Thrower, L. Hornekær and R. Martinazzo, "Bending the rules of PAH hydrogenation: the case of corannulene", Monthly Notices of the Royal Astronomical Society 519 (2023), 5567.*

104 **2023**, *P.J. Ollitrault, S. Jandura, A. Miessen, I. Burghardt, R. Martinazzo, F. Tacchino and I. Tavernelli, "Quantum algorithms for grid-based variational time evolution", Quantum 7 (2023) 1139.*

103 **2022**, *D. Campisi, T. Lamberts, N.Y. Dzade, R. Martinazzo, I.L. Ten Kate, A.G.G.M. Tielens, "Adsorption of Polycyclic Aromatic Hydrocarbons and C60 onto Forsterite: C–H Bond Activation by the Schottky Vacancy", ACS Earth and Space Chemistry, 6 (2022), 2009.*

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", 156 (2022) 194106.*

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", 156 (2022) 194106.*

100 **2022**, *R. Martinazzo and I. Burghadt, "Quantum dynamics with electronic friction", Physical Review Letters, 128 (2022) 206002.*

99 **2022**, *R. Martinazzo and I. Burghadt, "Quantum theory of electronic friction", Physical Review A, 105 (2022) 052215.*

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", 560 (2022) 111542.*

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, 237, (2022) 148-167.*

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 π 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, "Multiconfigurational 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.

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