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

10 Selected publications

1. **Sticking of atomic hydrogen on graphene**, *J. of Physics: Cond. Matter*, **30**, 283002 (2018), M. Bonfanti and S. Achilli and R. Martinazzo*.
   This invited topical review summarizes the experimental and theoretical efforts done in the last decade and aimed at understanding graphene hydrogenation at a microscopic level. The emphasis was put on the interplay between the adatom structures, their formation dynamics and the electric, magnetic and chemical properties of the carbon sheet.
2. **Full quantum dynamical investigation of the Eley-Rideal reaction forming H_2 on a movable graphitic substrate at T=0 K** , *Phys. Chem. Chem. Phys.*, **20**, 9779 (2018), M. Pasquini, M. Bonfanti and R. Martinazzo*.
   This work is the first study addressing the recombination of hydrogen atoms on a graphitic substrate including the lattice motion at a full quantum level. The correct description of this reaction and of its energy partitioning is crucial to assess the physics and the chemistry of the interstellar clouds.
3. **Hydrogen on silicene: like or unlike graphene?** , *Phys. Chem. Chem. Phys.*, **18**, 15654A (2016), M. Pizzochero, M. Bonfanti and R. Martinazzo*.
   This work reports on a theoretical investigation of silicene hydrogenation and a thorough comparison with the similar process in graphene. It was shown that, similarly to graphene, hydrogen adatoms act as strong resonant scatterers for charge carriers, and that, contrary to graphene, hydrogenation must proceed randomly under typical laboratory conditions, thereby resulting in degraded electric properties.
4. **Quantum dynamics of hydrogen atoms on graphene: II Sticking**, *J. Chem. Phys.*, **124**, 124704 (2015), M. Bonfanti, B. Jackson, K. H. Hughes, I. Burghardt and R. Martinazzo*.
   This work is the first fully converged quantum study of hydrogen atom sticking to graphene. It was shown that sticking is determined by a competition between barrier-crossing and energy transfer to the surface, and that a satisfactory description of the dynamics can be achieved with a simple impulsive model of a classical particle scattering off a quantum surface.

5. **Electron transport in carbon wires contacted to Ag electrodes: a detailed first principles investigation**, *Phys. Chem. Chem. Phys.*, **17**, 18413 (2015), P .Bonardi, S. Achilli, G. F. Tantardini and R. Martinazzo*.
   This work provides a chemically-oriented view of electron transport through carbon chains. Bonding between the electrodes and the capping species on the one hand, and between the latter and the carbon chains on the other hand, was shown to dramatically affect the transport properties of the molecular conductor.
6. **Structure and stability of hydrogenated carbon atom vacancies in graphene**, *Carbon*, **77**, 165 (2014), M. Caratelli, S. Casolo, G.F. Tantardini and R. Martinazzo*.
   This work reports on a detailed investigation of the hydrogenation of carbon atom vacancies in graphene, and its effects on the substrate properties. Comparison with transmission electron microscopy, scanning tunneling microscopy and muon-spin-resonance experiments showed that vacancies in graphene can be hydrogenated to various degree under ordinary conditions.
7. **Insights into hydrogen formation in space from ab initio molecular dynamics**, *Proc. Natl. Acad. Sci.*, **110**, 6674 (2013), S. Casolo, G.F. Tantardini and R. Martinazzo*.
   This work reports on an ab initio *molecular dynamics study of the (Eley–Rideal) recombination of hydrogen atoms on graphitic substrates. It was shown that the reaction dominates at interstellar medium conditions and alone may explain astronomical observations if the possibility of facile sticking at special sites (edges, point defects, etc.) of the surface of the dust grains is taken into account.*
8. **Universal Markovian reduction of Brownian particle dynamics**, *J. Chem. Phys. (Communication)*, **134**, 011101 (2011), R. Martinazzo*, B. Vacchini, K. H. Hughes, and I. Burghardt.
   This work reports, for the first time, an explicit construction of a Markovian embedding in a key physical problem, that of a Brownian particle obeying the generalized (classical or quantum) Langevin equation. It sparked the birth of the "reaction coordinate method", a useful tool in disparate disciplines like quantum thermodynamics, molecular electronics and the theory of orthogonal polynomials.
9. **Symmetry-induced band gap opening in graphene superlattices**, *Phys. Rev. B* **81**, 245420 (2010), R. Martinazzo*, S. Casolo, G.F. Tantardini.
   In this work it was shown by symmetry arguments and electronic-structure calculations that, contrary to widespread belief, it is possible to open a band gap in graphene without breaking its symmetry. The proposed structures, honeycomb superlattices of unitary defects, were shown to have new Dirac cones right close to the gapped region, and optimal gap size w.r.t. their length scale.
10. **Understanding adsorption of hydrogen atoms on graphene**, *J. Chem. Phys.*, **130**, 054704 (2009), S. Casolo, O. M. Lovvik, R. Martinazzo* and G. F. Tantardini.
    This work reports on a detailed investigation of the binding and barrier energies for sequential sticking of hydrogen atoms on graphene. The results were rationalized in light of Pauling's Resonating Valence Bond theory of chemical bond, and used to explain the formation of hydrogen dimer and cluster structures that had been long observed in graphene.

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