Matteo Bonfanti

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Generalities

Date of birth	December 2nd, 1984
Place of birth	Milano (Italy)
Nationality	Italian

Work Experience

November 2012 – present

Post-doctoral research fellowship at the Chemical Dynamics Theory Group of the Department of Chemistry at *Università degli Studi di Milano*
Supervisor: Dr. Rocco Martinazzo

- Research activity in Theoretical Physical Chemistry: simulations of dynamical processes of atomic hydrogen on graphitic (graphenic) surfaces, focusing on vibrational relaxation phenomena and reactive scattering (sticking). Simulations performed with molecular dynamics and quantum dynamics techniques. In particular, the research project involved the development of a molecular dynamics code from scratch for the simulation of the thermal equilibrium dynamics of the system (FORTRAN 90/95 – approx 21,700 lines).
- Co-supervision of bachelor and master thesis projects.

March 2013 – June 2013

Teaching assistance in Physics academic course
held by Prof. Fiorenza Quasso (*Dipartimento Di Scienze e Tecnologie Aerospaziali, Politecnico di Milano*)

- 48 hours of teaching assistance in the Physics course for undergraduate students in Engineering (exercises of mechanics, thermodynamics and electromagnetism)

February 2012 – November 2012

Post-doctoral research fellowship at the Theoretical Chemistry Group of Leiden University (The Netherlands)
Supervisor: Prof. Geert-Jan Kroes

- Research activity in Theoretical Physical Chemistry: simulation of reactive scattering of molecular hydrogen and methane from metal surfaces (H2 on Cu(111) and CH4 on Pt(111)). Study of the energetics of the reaction and of the dynamics at quantum level.

- Supervision of first year student internships in the theoretical chemistry group.

January 2009 – January 2012

PhD in Chemical Sciences at the University of Milan, in the Chemical Dynamics Theory Group of Prof. Gian Franco Tantardini.
Supervisors: Prof. Gian Franco Tantardini, Dr. Rocco Martinazzo

- Research activity in Theoretical Physical Chemistry: inclusion and effects of phonon degrees of freedom in the quantum dynamical simulation of atom and molecule scattering from surfaces. Results have been collected and defended in the doctoral thesis: "Reactions at surfaces: beyond the static surface approach in quantum dynamics"
- Visit to the Theoretical Chemistry group of Leiden University (NL), from September 2009 to September 2010. During this period, I extended the quantum reactive scattering code of Prof. Geert-Jan Kroes and Dr. Marc Somers for dealing with an additional degree of freedom describing the surface atoms motion (code in FORTRAN 90/95 - approx 97,700 lines)

April 2011 - May 2011

Tutoring in Numerical Analysis academic course

held by Prof. Claudio Verdi (*Dipartimento di Matematica*, *Università degli Studi di Milano*)

- 18 hours of tutoring in the Numerical Analysis course for undergraduate students in Chemistry. Resolution of chemical problems by numerical techniques in MATLAB environment.

February-March 2008
February-March 2009

Chemistry courses for high school students in preparation for university admission tests (10 hours in 2008, 12 hours in 2009), at the High School "*Liceo Scientifico Statale G. Falcone e P. Borsellino*", in Arese (Italy)

Education

2009 – 2011

PhD in Chemical Sciences at the University of Milan
PhD Thesis: "*Reactions at surfaces: beyond the static surface approach in quantum dynamics"* (defended on 16th January 2012)
Supervisors: Prof. Gian Franco Tantardini, Dr. Rocco Martinazzo

- Training to research activity, also by attending courses and literature seminars.
- Advanced knowledges of Physical Chemistry and Theoretical Chemistry. Among others, I attended some courses the Physics Department of *Università degli Studi di Milano* to improve my understanding of statistical mechanics: "Computational Physics" held by Prof. Davide Galli for PhD students (30 hours) and "*Meccanica Statistica*" (Statistical Mechanics) held by Dr. Bruno Bassetti for master students in Physics (40 hours).

2006 - 2008	**Master Degree in Chemical Sciences**, at the University of Milan, *summa cum laude*. (24th October 2008) Dissertation thesis: "*Study of the relation between hydrogen affinity and magnetic properties in Polycyclic Aromatic Hydrocarbons*" . Supervisors: Prof. Gian Franco Tantardini, Dr. Rocco Martinazzo. • Advances knowledges in Physical Chemistry: thermodynamics and statistical mechanics, theory of matter, solid state physics, quantum and theoretical chemistry.
2003 - 2006	**Bachelor Degree in Chemistry**, at the University of Milan, *summa cum laude*. (26th October 2006) Dissertation thesis: "Ab Initio study of H-coronene interaction modelling physisorption of atomic hydrogen on graphite". Supervisors: Prof. Gian Franco Tantardini, Dr. Alessandro Ponti, Dr. Rocco Martinazzo. • Basic knowledges in Chemistry, Physics, Math and Computer Science. General understanding of the various branches of Chemistry: Physical, Organic and Inorganic Chemistry
1998 - 2003	**High School Diploma** at the "Liceo Scientifico Piero Bottoni", Milan, Italy. Full marks.

Languages

Italian	mother tongue
English	fluent
Dutch and Spanish	basic

Computer skills

Operating systems	installation, administration and use of *Linux* (Red Hat distributions in particular) and *Windows* systems
Programming	*Fortran 90-95*, *Python*, basic knowledge of *C* and *C++* Unix shell scripting (*csh*, *bash*, *awk*) Parallel computing libraries (*OpenMP*, *MPI*) *Subversion* and GIT revision control system
Scientific software	Quantum Chemistry packages (*GAMESS*, *Gaussian*, *MolPro*, *VB2000*) Density Functional Theory codes (*DaCapo*, *Siesta*) Quantum Wavepacket Dynamics codes (*MCTDH*)
Graphic software and data visualization	*ParaView, Gimp, Inkscape, xmGrace, Xfig* rendering of molecular structures with *POV-Ray* and *Tachyon*
Editors and utilities	*MS Office* and *OpenOffice*, *Latex*/*Lyx*, *Beamer*

Courses, Conferences and Schools

June 2014	**School "Introduction to Scientific and Technical Computing C++"**, organized by CINECA, Segrate, Milano (Italy), June 25th-27th 2014
April 2013	**School "Introduction to C Programming Language for Scientific Applications"**, organized by CINECA, Segrate, Milano (Italy), April 22nd-23rd 2013
April 2013	School "**Rome school on Open Systems and the Quantum-Classical Boundary**", Rome, April 8th-12th, 2013
November 2012	Workshop "**Dynamical Phenomena at Surfaces: The role of complexity**", Lorentz Center, Leiden (NL), November 26th-30th, 2012 **Poster**: "*7D quantum dynamics of H2 scattering on Cu(111)*"
June 2012	**Spectroscopy and Theory Study Group Meeting**, Utrecht (NL), June 15th, 2012
April 2012	Conference **"High dimensional quantum dynamics: challenges and opportunities"** Birmingham (UK), from April 11th to 13th 2012. **Poster**: "*Vibrational Sudden Approximation for Lattice Motion in H2/Cu(111) Quantum Reactive Scattering*"
December 2010	Conference **"Elementary Reactive Processes at Surfaces 2010",** Talence (France), from November 30th to December 3rd, 2010. **Poster**: "*The effect of surface motion on H_2 dissociation on Cu(111)*"
September 2010	Conference **"Passion for Knowledge"** held at Kursaal Centre of San Sebastian (Spain), from September 28th to October 1st 2010. **Poster**: "*The effect of surface motion on H_2 dissociation on Cu(111)*"
February 2010	**Scientific meeting on Chemistry related to Physics & Material Sciences** organized by the Netherlands Organisation for Scientific Research (NWO), at Veldhoven (NL), February 15th-16th 2010. **Poster**: "*Modelling surface motion in H_2 +Cu(111) quantum dynamics*"
August 2009	**Gordon Conference on Dynamics at Surfaces**, at Proctor Academy in Andover, New Hampshire (USA), August 9th-14th 2009. **Poster:** "*The influence of the substrate model in the Eley-Rideal hydrogen formation on graphite*"
June 2009	**InGAP-NANOCAT Summer School** International Summer School on Molecular and Supramolecular Approach to Nano-Designed Catalysts with Industrial Relevance, in Trondhein (Norway), June 21st-26th 2009. **Poster**: "*Hydrogen affinity and magnetic properties of small Polycyclic Aromatic Hydrocarbons*"
March 2009	**Nanoscale modelling of new molecular experiments**: theoretical and computational simulations, Interdisciplinary Workshop - 6th March 2009 at Accademia dei Lincei, Roma. **Poster**: "*Hydrogen affinity and magnetic properties of small polycyclic aromatic hydrocarbons*"
February 2008	**School on FORTRAN 90** for intense scientific computation, Consorzio Interuniversitario Lombardo per l'Elaborazione Automatica (Cilea), Segrate, Milano (Italy), February 19th-21st 2008

Visits

September 2009 - September 2010	**Guest student at the University of Leiden** in the Theoretical Chemistry Group, under the supervision of Prof. Geert-Jan Kroes.

Research Grants and Projects

2014	Principal investigator of a **development project within the LISA initiative** of the CINECA Italian supercomputing facility for the parallelization of an *Ab Initio* Molecular Dynamics code, developed to perform equilibrium quantum simulation by means fo Ring Polymer Molecular Dynamics.
2013-2014	Collaborator of two **production projects within the LISA initiative** of the CINECA Italian supercomputing facility. Aim: perform electronic structure calculation with SIESTA on a massively parallel machine (the Fermi supercomputer, an IBM BlueGene/Q)
2012	Collaborator of a **PRACE preparatory project** for testing the parallelization of the quantum wave-packet code on a large parallel machine (Tier-0 Curie supercomputer at the TGCC by CEA)
2010	**LLP/Erasmus Grant**, supports to the visit at the Theoretical Chemistry Group of Prof. Kroes at Leiden Universiy

Publications

1	M. Bonfanti, G. F. Tantardini and R. Martinazzo *Adiabatic Potential Energy Surfaces for the Low Energy Collisional Dynamics of $C^+(_2P)$ Ions with H_2 Molecules* The Journal of Physical Chemistry A; **118**, *6595-6603* (2014).
2	A. Mondal, M. Wijzenbroek, M. Bonfanti, C. Diaz, G.-J. Kroes *Thermal Lattice Expansion Effect on Reactive Scattering of H_2 from Cu(111) at T_s = 925 K* The Journal of Physical Chemistry A; **117**, *8770-8781* (2013).
3	M. Bonfanti, M.F. Somers, C. Dìaz, H.F. Busnengo and G.J. Kroes *7D Quantum Dynamics of H_2 scattering from Cu(111): the accuracy of the phonon sudden approximation* Zeitschrift für Physikalische Chemie, **227**, *1397-1420* (2013).
4	M. Bonfanti, G.F. Tantardini, K.H. Hughes, R. Martinazzo and I. Burghardt *Compact MCTDH wave functions for high-dimensional system-bath quantum dynamics* Journal of Physical Chemistry A, **116**, *11406* (2012)
5	M. Bonfanti, S. Casolo, G. F. Tantardini, A. Ponti and R. Martinazzo *A few simple rules governing hydrogenation of graphene dots* Journal of Physical Chemistry, **135**, *164701* (2011)

6 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
Physical Chemistry Chemical Physics, **13**, *16680-16688* (2011)

7 M. Bonfanti, C. Dìaz, M. Somers, G.J. Kroes
Hydrogen dissociation on Cu(111): the influence of lattice motion.Part I
Physical Chemistry Chemical Physics, **13**, *4552-4561* (2011)

8 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**, *14545–14553* (2009)

9 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**, *5825* (2007)

References

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