Proposal for a Psi-k Workshop (cosponsored by Univ. Roma "La Sapienza")

Progress in ab initio modelling of biomolecules: towards computational spectroscopy

Location: Department of Physics, University of Roma "La Sapienza"

Dates: 2-4 April 2007

Organisers
L. Guidoni
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Abstract
First principle electronic structure calculations are an emerging theoretical and computational tool to unravel mechanistic details of biological systems. Its rapid development is opening the avenue to the study of increasingly complex systems and, at the same time, to the possibility to perform affordable and accurate calculations of structural, dynamical and spectroscopic properties of biomolecules. The aim of the proposed workshop is to give to the researcher who are active in this field the opportunity to exchange and integrate their expertise with the specific target of merging together different techniques, which might help bring the calculations closer to the experiments.

Scientific Summary
In the last few decades biology has been undergoing a revolution that is leading it closer to the microscopic atomic scale. Experimentally determined 3D structures of biological molecules refined with atomic resolution are indeed becoming available and they represent nowadays a fundamental and un-replaceable starting point to understand the molecular interactions in living matter. At the same time many other experimental techniques are expanding their predictive capabilities to the point that it is now feasible the study of single molecules properties, such as structural, optical, magnetic, and dynamical properties, with increasing resolution.
In order to go beyond speculative conjectures or qualitative interpretations of this exponentially increasing amount of data, it is constantly necessary to develop new computational tools to properly simulate these systems and correctly describe their molecular properties and dynamics at the atomistic level. In this respect, in the last ten years, first principles calculations have opened a venue in both the study of increasingly complex systems and the possibility of a direct quantitative comparison between the calculated molecular properties and the biochemical experiments.

The investigation of biologically active molecules, such as proteins and DNA, from first principles, however poses its own unique set of problems. Biological systems present an extremely high degree of complexity. First of all, biomolecules like proteins may contain several hundreds of amino acids, i.e., thousands of atoms. Secondly, biological processes occur in aqueous solution and span millisecond or even seconds time scales. In addition, very often solvent molecules have an active role and have to be explicitly considered. Furthermore, dynamical effects both on short and long time scales are extremely important and must be taken into account. Therefore, the overall accuracy

and predictive capability of computational models for biological systems are limited by (*i*) the accuracy to which relevant phase space regions are sampled, (*ii*) the degree to which the microscopic system on the computer reflects the macroscopic system in nature, and, in addition, (*iii*) the accuracy to which molecular properties and interaction forces are described.
One of the most critical challenges in the near future is to reach a high accuracy in the quantum description of biomolecules so that it would be possible to reliably predict in silico many molecular properties starting from structural basis only. The comparison between simulations and data obtained by experiments (such as chemical kinetics, NMR, EPR, optical and vibrational spectroscopy) will allow us to better understand the function and the structure/function relationships of biomolecules.

The aim of this workshop is to give the researchers who are active in this field the opportunity to exchange and integrate their expertise with the specific target of merging together different techniques, which might help bring the calculations closer to the experiments. The meeting will benefit from the participation of several Psi-k head working groups, which will offer their long expertise in the field of electronic structure computation. The participation of few experimental groups (supported by external funds) is also scheduled with the aim to bring the theoretical physicist community closer to experimental biophysics to envisage common strategies for the development of a "quantitative computational molecular biology".

Many theoretical and technical challenges are currently preventing in many cases computer modeling to be used the quantitative comparison with the experiments. A number of crucial technical problems and methodological issues have been arising in recent years, and a strong effort is currently undertaken to their overcome. Among the number of issues related to the study of biological systems, the workshop will focus on the ensuing major issues and problems.

1. *Excited states and electron transfer.* A variety of biological processes, such as vision and photosynthesis, are guided and regulated by electronic excitations of light-sensitive protein chromophores. Absorption and emission spectra as well as time-resolved optical properties of these molecules can be monitored accurately by experiments directly in both their complex biological environment and in the gas phase. Although a large quantity of spectroscopic data is nowadays available for a large number of photosensitive systems, such as rhodopsin, fluorescent proteins and photosystems complexes, a quantitative treatment of the electronic structure of large molecules in their excited states is still a big challenge in first principles methods.
2. *Computational spectroscopy*. Beside optical spectroscopy, a plethora of other spectroscopic techniques, including NMR, IR, Raman, Mossbauer, electronic spectroscopy, EXAFS etc. is crucial to experimentally characterize structure, dynamics and function of biomolecules. The calculation of several of these quantities for large macromolecules remains however a major challenge for theoreticians, especially because these quantities often depend on the environment in a quite intricate way.
3. *Computational Biophysics beyond DFT.* DFT-based methods, which have the advantage of being rather computationally-cheap, often fail when dealing with excited states and charge transfer. On the other hand, higher level calculations become extremely expensive for large systems, and are applicable, up to now, only to a limited number of systems, like solids (e.g., GW corrections) or small molecules in vacuo (e.g., quantum chemistry methods, like CAS-SCF or CAS-PT2 and, more recently, QMC). The development of novel techniques and the integration and improvements of the ones currently available is therefore a crucial step for the theoretical biophysics community to extend current ab intio approaches to more complex and realistic biological systems.

Location
The workshop will be held at the Department of Physics of the University "La Sapienza" in Rome, April 2007 which kindly offers lecture rooms and logistic support. The location can also benefit from the fact that Rome airports are daily connected with all main European cities by low cost flights (Air Berlin, Blue-Express, EasyJet, Germanwings, Meridiana, Ryanair, Sky Europe, Transavia, Virgin Express, and many others).

Organization
The workshop is structured in six plenary sessions, spanned over three days. The program of the workshop covers the following main topics:

- Linear scaling ab initio methods
- Time dependent Density Functional Theory: flaws and improvements
- High level ab initio approaches to excited states
- Charge transfer processes in (bio)molecules
- Calculation of IR, Raman and NMR spectra of drug/protein complexes
- Electron Transfer
- Hybrid methods

Tentative list of speakers:

Theory/Computation

W. Andreoni	IBM Research Zurich, Switzerland
E.J. Baerends	Vrije Universiteit, Amsterdam, The Netherlands
F. Buda	Univ. Leiden, the Netherlands
P. Carloni*	SISSA, Trieste, Italy
G. Ciccotti*	Dipartimento di Fisica, Universita' , Italy
L. Colombi Ciacchi*	Fraunhofer Institut für Werkstoffmechanik, Freiburg, Germany
C. Dellago	University of Vienna, Austria
C. Filippi*	Univ. Leiden, the Netherlands
E.K.U. Gross	Freie Universität Berlin, Germany
M. Iannuzzi*	University of Zürich, Switzerland
M. Kaupp	Universitaet Warzburg, Germany
D. Marx	Ruhr-Universitaet Bochum, Germany
R. A. Mathies	University of California, Berkeley, USA
C. Molteni*	Imperial College, London, United Kingdom
M. Olivucci	Univ. of Siena, Italy
O. Pulci*	Università di Tor Vergata, Roma, Italy
U. Röthlisberger	EPFL, Losanne, Switzerland
A. Rubio	Universidad del Pais Vasco, San Sebastian, Spain
M. Scheffler	Fritz Haber Institute, Berlin, Germany
D. Sebastiani*	MPI for Polymer Research, Mainz, Germany
A.L. Sobolewski	Polish Academy of Sciences, Warszawa, Poland
M. Sprik	Univ. of Cambridge, United Kingdom
I. Tavernelli*	EPFL, Lausanne, Switzerland
V. Tozzini*	NEST-CNR-INFM, Pisa, Italy
J. Vandevondele*	ETH Zürich, Switzerland
R. Vuilleumier*	Università Pierre et Marie Curie, Paris, France

Experimentalists (expenses for non-European speakers will be covered by non-ESF funds)

V.Y. Orekhov	Swedish NMR Centre Goeteborg University, Sweden
H.B. Gray	Beckman Institute, California Institute of Technology Pasadena, USA
M.S. Helfand*	Case Western Reserve University, University Hospitals of Cleveland Cleveland, Ohio, USA.
R. Mathies	Univ. of California, Berkeley, USA
S.B. Nielsen	Univ. of Aarhaus, Denmark

* Confirmed Speaker

Leonardo Guidoni – Curriculum Vitae

Personal Data

Name	Leonardo Guidoni
Date of Birth	8th of January 1972
Present Address	Università di Roma "La Sapienza", Dipartimento di Fisica Edificio Fermi, stanza 111 P.le Aldo Moro 5, 00185, Roma, Italy Tel: +39 06 4991 3314 Fax: +39 06 446 3158
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Education and Fellowships

Aug-Sep 2006	Invited Professor at the University of Leiden, The Netherlands.
Aug-Sep 2005	Invited Professor at the Swiss Federal Institute of Technology in Lausanne, Switzerland.
Dec 2004-	"Brain Drain" Professorship in Computational Biophysics and Biochemistry at the department of Physics of the University of Rome "La Sapienza".
Jul 2002	Post-doctoral position at the Swiss Federal Institute of Technology in Lausanne, Institute of Molecular Chemistry and Biology, in the group of Prof. U. Röthlisberger.
Nov 2000	Post-doctoral position at the Swiss Federal Instutute of Technology in Zürich, Department of Inorganic Chemistry, in the group of Prof. U. Röthlisberger.
Oct 2000	Doctor Philisophiæ degree *cum laude* in Theory of Condensed Matter at the International School for Advanced Studies of Trieste. Thesis: *Theoretical Studies on the KcsA Potassium Channel.* Supervisors: P. Carloni, V.Torre.
1997	Civilian service.
Jul 1996	Degree in Physics at Università degli Studi di Roma "La Sapienza" with first class honors (mark 110/110 *cum laude*). Thesis: *Spin system with orbital degeneracy: lattice Monte Carlo.* Supervisors: G.B. Bachelet, G. Santoro, S. Sorella.

Languages Italian (mother tongue), English (fluent).

Teaching activity

Oct 2006-Dec 2007	Course "Simulazione Atomistica (Laurea Specialistica)" at the University of Rome "La Sapienza".
Mar 2006-May 2006	Course "Fisica Teorica della Struttura della Materia" for the Phd in Physics at the University of Rome "La Sapienza".
Apr 2006-Jun 2006	Course "Esercitazioni di Meccanica dei Sistemi Continui per Fisica (Laurea Triennale)" at the University of Rome "La Sapienza".
Jan 2006-Mar 2005	Course "Esercitazioni di Meccanica Classica per Fisica (Laurea Triennale)" at the University of Rome "La Sapienza".
Mar 2005-May 2005	Course on *Molecular Dynamics* for the Phd in Physics at the University of Rome "La Sapienza".
Oct 2002 – Jan 2003	Assistant at the practical computer training during the course "Computational chemistry" at the Swiss Federal Institute of Technology in Lausanne.
Sep-Oct 2002	Supervisor of the semester student Pirmin Ulmann at the Swiss Federal Institute of Technology in Lausanne.

Refereeing

I am referee for the following international journals: *Biophysical Journal; Proteins, Structure Function and Genetics; Journal of Biomolecular Structure and Dynamics; Future Generation Computer Systems.*

Talks and seminars

Jul 2006	Leiden, The Netherlands	Contributed talk to the Psi-k workshop 'Progress in ab initio modeling of biomolecules: methods and applications': *"Absorption Spectra by QMC/MM"*
May 2006	Bertinoro, Italy	Invited talk to the workshop 'Perspectives on Science and Engineering Driven Supercomputing': *"High Performance Computing in Biophysics and Biochemistry"*
May 2006	Lyon, France	Cotributed talk to the CECAM Workshop 'New developments for first principles MD simulations in condensed matter and Molecular physics': *"Absorption Spectra in Solution by QMC/MM Simulations"*
May 2006	Gaeta, Italy	Invited talk to the 5th Workshop on Molecular Theories and Simulations: *"Calculating absorption spectra of biomolecules: QM/MM, TDDFT and Quantum Monte Carlo"*
Feb 2006	Roma, Italy	Contributed talk to the Conference ABR06: "First Principles Quantum Mechanics/Molecular Mechanics (QM/MM) Simulations of Biological Systems"
Oct 2005	Rimini, Italy	Invited talk to the 3rd National Congress on Chemistry of Biological Systems: "Quantum Monte Carlo as high accuracy computational method for Biological Chemistry"
Sep 2005	Scwäbisch Gmünd, Germany	Contributed talk to the Psi-k 2005 Conference: "*Absorption spectra in solution: combining Quantum Monte Carlo with Car-Parrinello Dynamics*"
Jul 2005	Roma, Italy	Contributed talk to the European Symposium on Organic Reactivity: *"Electronic reaction coodinates"*
May 2005	Gaeta, Italy	Invited talk to the 4th Workshop on Molecular Theories and Simulations: *"Ab initio Quantum-Mechanics/Molecular Mechanics Simulations of biological systems"*
Sep 2004	Genova, Italy	Contributed talk to the Conference on Computational Physics: *"Accelerating Chemical Reactions in mixed Quantum/Classical Simulations by Biasing Molecular Orbitals"*
Feb 2003	Trieste, Italy	Invited Seminar at the Democritos INFM Center by Prof. Paolo Carloni: *"Molecular Mechanisms of light Detection in Rhodopsin"*.
Nov 2003	Modena, Italy	Invited Seminar at the S3 INFM Center by Prof. Elisa Molinari: "*Classical and Mixed QM/MM dynamics in biological and biomimetic systems*".
Oct 2003	Lausanne, Switzerland	Contributed talk to the *Swiss Chemical Society Fall Meeting 2003*: "Driving Chemical Reactions via Biases of Molecular Orbitals".
Feb 2003	Frascati, Italy	Contributed talk to conference *Advances in Experimental and Theoretical Methods for Biological Application of Synchrotron Radiation (BioSR)*: "QM/MM Simulations of Rhodopsin: Insights into the Early Steps of Light Detection in the Eye.
Nov 2002	Bern, Switzerland	Biochemistry Seminar at the *University of Bern*, invited by Prof. B. Erni: "Exploring biological systems by quantum and molecular mechanics simulations".
Nov 2002	Basel, Switzerland	Physical Chemistry Seminar at the *University of Basel*, invited by Prof. H. Huber: "Ab initio and molecular mechanics simulations of biological systems".
Apr 2002	Roma, Italy	Contributed talk to the conference *Acta Biophysica Romana 2002*: "Simulating the molecular mechanisms of membrane proteins: ionic channels and photoreceptors".
Sep 2001	Manno, Switzerland	Contributed talk at the *CSCS users day*: "Mixed Quantum/Classical QM/MM Car-Parrinello simulations in biological sistems".
Jun 2001	Roma, Italy	Contributed talk to the *National Conference of Physics of Matter*: "Modeling permeation and blocking in potassium channels".
Mar 2001	Roma, Italy	Seminar at the physics department of *Universitá di Roma "La Sapienza"*, invited by Prof. A. Congiu-Castellano: "Ionic

		channels: permeation and blocking mechanisms".
Feb 2001	Boston, MA (USA)	Contributed talk to the *Biophysical Society 45th Annual Meeting* (*Biophys. J.* 80, A175 (2001)): "Barrier crossing in the selectivity filter of KcsA potassium channel".
Oct 2000	Parma, Italy	Invited talk at the *XV Meeting of the Italian Society of Pure and Applied Biophysics (SIBPA 2000)*: "Theoretical studies on the KcsA potassium channel ".
Mar 2000	Rome, Italy	Seminar at the physics department of *Universitá di Roma "La Sapienza"*, invited by Dr. A. Giansanti: "Ionic channels: from the first crystal to molecular dynamics".
Feb 2000	New Orleans, LA (USA)	Contributed talk to the *Biophysical Society 44th Annual Meeting* (*Biophys. J.* 78, A138 (2000)): "Hydration and dynamics of the K^+ channel".
May 1999	Trieste, Italy	Contributed talk at the *Workshop on Phototransduction and Chemotransduction organized by the consortium of E.C. Biotech Project*: "The KcsA potassium channel: microscopic and dynamical properties".
Feb 1999	Charlottesville, VA (USA)	Seminar at the *University of Virginia Health Sciences Center*, invited by E. Perozo: "K^+ channel tetrameric stability explored by molecular dynamics simulations".
Feb 1999	Baltimore, MD (USA)	Contributed talk to the *Biophysical Society 43rd Annual Meeting* (*Biophys. J.* 76, A153 (1999)): "K^+-potassium channel interactions explored by molecular dynamics simulation".
Nov 1998	Miami, FL (USA)	Contributed talk to the *43rd Annual Conference on Magnetism and Magnetic Materials*: "Spin gap in low-dimensional Mott insulators with orbital degeneracy".

Awards

Jan 2003-Sep 2004	Glarus, Switzerland	Velux Stiftung post-doctoral fellowship at The Swiss Federal Institute of Technology in Lausanne.
Jul 2002	Lugano, Switzerland	Best Poster Presentation Award *at the 6th World Congress of Theoretically Oriented Chemists.*
Jun 2000	Genova, Italy	Young author award *of the National Conference on Physics of Matter.*

Selected Publications of the last 5 years

L. Guidoni, P. Carloni, Potassium permeation through the selectivity filter of the KcsA channel: a density functional study, *Biochim.Biophys.Acta* **2002,** *1563* 1-6.

U. F. Rohrig, L. Guidoni, U. Rothlisberger, Early steps of the intramolecular signal transduction in rhodopsin explored by molecular dynamics simulations, *Biochemistry* **2002,** *41* 10799-10809.

L. Guidoni , K. Spiegel, M. Zumstein, U. Rothlisberger, 'Green' Oxidation Catalysts: Computational Design of High-Efficiency Models of Galactose Oxidase, *Angewandte Chemie, Int.Ed.* **2004,** *43* 3286-3289.

U. F. Rohrig, L. Guidoni , A. Laio, I. Frank, U. Rothlisberger, A molecular spring for vision, *J.A.C.S.* **2004,** *126* 15328-15329.

L. Guidoni , U. Rothlisberger, Scanning reactive pathways with orbital biased molecular dynamics, *J.C.T.C.* **2005,** *1* 554-560.

Simone Raugei - Curriculum Vitae

Simone Raugei was born in Florence in May 28th 1970. He got his PhD in Chemistry at the University of Florence in 1999 with a Thesis on the application of theoretical models to the study of chemical reactions and phase transitions. During his PhD he visited for a long period the Max Plack Institute for solid state physics in Stutgart, Germany (Prof. M. Parrinello's group). In 2000 he moved to the Center for Molecular Modeling, University of Pennsylvania, Philadelphia, USA (Prof. M. L. Klein's group) where he carried out studies of catalytic processes. In 2002 he moved to SISSA, Trieste, Italy as “Ricercatore a contratto” (Prof. Carloni's group). His research efforts are focused on the development, implementation and application of a variety of state of the art computational techniques to investigate the intricate relationships between structure and function in biological systems. He is co-author of more than 30 papers published on scientific journals of international renown and he has been invited to over than 10 international meetings.

He also co-organized with A.Magistrato and P. Carloni a joint INFM Democritos/PSI-k Network workshop on *ab initio modeling of biological systems* held at SISSA in May 15-16, 2004.

Selected publications

V. Carnevale, **S. Raugei**, C. Micheletti, and P. Carloni.
Convergent dynamics in the protease enzymatic superfamily.
J. Am. Chem. Soc. **128**, 9766 (2006).

I. Ivanov and B. Chen and **S. Raugei** and M. L. Klein.
Relative pKa’s from first principles molecular dynamics: the case of histidine deprotonation.
J. Phys. Chem. B **110**, 6365 (2006).

S. Raugei and P. Carloni.
Structure and function of vanadium haloperoxidases.
J. Phys. Chem. B **110**, 3747 (2006).

M. Dal Peraro, **S. Raugei**, P. Carloni and M. L. Klein.
Solute-Solvent Charge Transfer in Aqueous Solution.
ChemPhysChem **6**, 1719 (2005).

S. Raugei and M. Cascella and P. Carloni.
A proficient enzyme: Insights on the mechanism of orotidine monophosphate decarboxylase from computer simulations.
J. Am. Chem. Soc. **126**, 15730 (2004).

Curriculum Vitae of Michele Cascella

General information:

Name: Michele Cascella
Nationality: Italian
Date of birth: December, 11, 1975
Place of birth: Santa Maria Capua Vetere (CE), Italy
Mother tongue: Italian

Present Address:

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Current Position:

Post-doctoral position at EPFL, Lausanne, in prof. Ursula Roethlisberger's group.

Education and Qualifications:

- October 1994- Summer 1999: undergraduate studies in Chemistry at Università degli Studi ``La Sapienza", Rome.
- April 2000: Degree in Chemistry "cum Laude". Thesis: Vibrational excitations of polyatomic gases induced by electron scattering. Supervisor: Prof. Francesco A. Gianturco.
- November 2000 - September 2004: Ph.D. student at the International School for Advanced Studies (SISSA/ISAS), Trieste.
- October 2004: Ph.D. in statistical and biological physics. Thesis: Evolutionarily-conserved functional mechanics across pepsins and retropepsins. Supervisor: Prof. Paolo Carloni.

Foreign Languages:

- English; proficient.
- French; fair.
- Spanish; reading.

Selected publications in refereed journals:

M. Cascella, S. Raugei and P. Carloni
"Formamide hydrolysis investigated by multiple steering ab-initio molecular dynamics";
J. Phys. Chem. B, 108:369-375 (2004).

P. Vidossich, M. Cascella and P. Carloni
“Dynamics and energetics of water permeation through the aquaporin channel";

Proteins: Structure, Function and Bioinformatics, 55:924-931 (2004).

M. Cascella, C. Micheletti, U. Rothlisberger and P. Carloni
"Evolutionarily-conserved functional mechanics across pepsin-like and retroviral aspartic proteases";
J. Am. Chem. Soc., 127:3734-3742 (2005).

M. Neri, C. Anselmi, M. Cascella, A. Maritan and P. Carloni
"Coarse-grained model of proteins incorporating atomistic detail of the active site";
Phys. Rev. Lett., 95:218102 (2005).

V. Garbuio, M. Cascella, L. Reining, R. Del Sole and O. Pulci
"Ab-initio calculation of optical spectra of liquids: many-body effects in the electronic excitations of water";
Phys. Rev. Lett., in press.

Contributions at Conferences:

- "Water exchange reaction at alkali ions", poster presented at "FHI workshop" (August 2001, Berlin, D)
- "Ab initio Molcular Dynamics study of Formamide hydrolysis", poster presented at the 5th "WATOC" congress (Special award winner) (September, 2002, Lugano, CH)
- “Enzymatic Mechanism of aspartic proteases from first principles", poster presented at the Conference on "Ab-initio Electron-Excitations Theory: Towards Systems of Biological Interest", (September 2003, San Sebastian, E)
- "Electron Transfer Properties of Azurin from Pseudomonas Aeruginosa by Hybrid QM/MM Molecular Dynamics Simulations", Oral contribution to the Fall Meeting of the Swiss Chemical Society, (October 2006, Zuerich, CH)

Other participations at Workshops and Conferences:

- Spring College on ``Electronic Structure Approaches to the Physiscs of Materials", (May-June 2000, Trieste, I)
- International Workshop on "Protein Folding, Structure and Design", (June 2001, Trieste, I)
- Adriatico Research Conference on ``Interaction and Assembly of Biomolecules" (August 2001, Trieste, I)
- College on Biophysics: "From Molecular Genetics to Structural Biology", (October 2001, Trieste, I)
- Winter College on "Numerical Methods in Electronic Structure Theory", (January 2003, Trieste, I)
- INFM Conference on "New Frontiers in Nano-Biotechnology: Monitoring Protein Function with Single-Protein Resolution", (July 2003, Trieste, I)
- "Workshop on Biopolymers" (May-June 2005, Trieste, I).

Seminars:

- June 2002: Invited talk in Prof. G.B. Bachelet group at the University of Rome "La Sapienza". *"Simulating molecular systems in aqueous solution by Car-Parrinello Molecular Dynamics"*

- April 2004: invited talk in Prof. M.L. Klein group at the University of Pennsylvania, Philadelphia. *"Conserved functional mechanics across Pepsins and Retropepsins"*
- July 2004: invited talk at the department of mathematical biology at the National Institue of Medical Research, London. *"Conserved functional mechanics across Pepsins and Retropepsins"*
- September 2006: invited talk at the first informal CMM QM/MM Workshop, Philadelphia, USA. *"Electron Transfer Properties of Azurin from Pseudomonas Aeruginosa by Hybrid QM/MM Molecular Dynamics Simulations"*.