Dr. LAURA GAGLIARDI

PERSONAL DATA

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References:
Professor Rudolph Marcus, California Institute of Technology, email: ram@caltech.edu
Professor Björn O. Roos, Lund University, email: bjorn.roos@teokem.lu.se
Professor Pekka Pyykkö, University of Helsinki, email: pyykko@chem.helsinki.fi
Professor Christopher J. Cramer, University of Minnesota, email: cramer@pollux.chem.umn.edu
Professor Kimihiko Hirao, Tokyo University, email: hirao@qcl.t.u-tokyo.ac.jp

1 Education and Curriculum vitae

1982-1987: Higher Education at Classical Liceum ”L. Galvani”

July 1987: High school degree: 60/60 (Maximum mark)

1987-1992 First degree education at the Faculty of Industrial Chemistry, University of Bologna

November 1992: Laurea in Industrial Chemistry: 110/110 cum laude (Maximum mark), Faculty of Industrial Chemistry, University of Bologna

1993-1996 PhD in Theoretical Chemistry, University of Bologna

November 1993: winner of the award ’Toso-Montanari’ University of Bologna for the student with the highest mark of the year

July 1997: PhD Examination in Theoretical Chemistry, University of Bologna

1997-1998: Research Associate in the group of Professor N.C. Handy, University of Cambridge UK

1999-2000: Research Fellowship at the Department of Physical and Inorganic Chemistry, University of Bologna

January 2001-July 2002: Research and Lecture Contract at the Department of Chemistry G. Ciamician, University of Bologna

Since July 2002: Permanent position as Assistant Professor at the University of Palermo

October-November 2003: Visiting Professor at the University of Tokyo (group of Professor Hirao).

July 2004: Winner of the 2004 award of the International Academy of Quantum Molecular Science

August 2004: Visiting Professor at the University of Tokyo (group of Professor Hirao).

2 Research Activity

1992

Graduation project with a thesis on "Near UV high resolution electronic spectrum of 1H-Benzotriazole" [1].

1993-1996

PhD in quantum chemistry with a thesis on "Configuration Interaction methods for the study of molecular properties". (Supervisor Professor G. L. Bendazzoli). During the PhD I implemented a Full CI code and used Full CI and highly correlated methods to study properties of small molecules like BH, Be_2, Li_2 [2]-[4],[6],[7] [**?**].

Part of the PhD was carried out in the group of Professor B.O. Roos, Lund, where I specialized in the use of CASSCF and CASPT2 approaches to study hypothetical nitrogen clusters, which can be considered as prototypes of high energy density materials [5],[8],[9].

1997-1998

Contract as a Research Associate in the group of Professor N.C. Handy, Cambridge, UK, within a TMR fellowship. I worked together with other five young scientists (senior scientist Dr. Andrew Willetts) on a project partially sponsored by British Nuclear Fuels, UK, with the aim of developing a new DFT program intended for the study of heavy element compounds.

Specifically I worked on the inclusion of relativistic effects with two component methods and treatment of spin orbit effects [10],[12],[17]. I also performed most of the applications on actinide chemistry [11],[13],[14]. This period allowed me to enter into what nowadays is one of my main areas of expertise, namely heavy element quantum chemistry.

1999-2000

Research Fellowship at the Department of Physical Chemistry, University of Bologna.

I continued to work in the area of heavy element chemistry with the use of DFT techniques, being the only person carrying on this research in the group [18]. I studied plutonium and uranium compounds of interest for the nuclear industry [20] and actinide compounds of spectroscopical interest like uranium and thorium tetrahalides [19].

In the meanwhile I realized the necessity of treating actinide and heavy element compounds with multiconfigurational methods, especially when they have an open shell nature and they cannot be extensively described with a single reference method like DFT. I thus contacted the Lund group, which has a long tradition in multiconfigurational methods for the study of organic chemistry and transition metal chemistry, and suggested to set up a new project on actinide chemistry. This would involve the Lund expertise in treating correlation and my expertise on heavy element

chemistry and relativistic effects. In collaboration with the Lund group, I started a systematic benchmark of DFT for heavy element systems towards wave function based methods [21]. I have also started a collaboration with the group of Professor J.M. Dyke, Southampton, UK. Professor Dyke is a distinguished spectroscopist who, among other systems, studies also small actinide molecules in the gas phase [19]. This has allowed me to focus on applications of spectroscopical interest.

As regards method developments, I continued a project started in Cambridge on the inclusion of spin-orbit effect in a DFT framework [22]. I have also worked on new methods for numerical integration [24] in collaboration with the Lund theoretical chemistry group.

2001 -2004

I worked in the group of Professor G. Orlandi in Bologna in the period 2001-2002. One of the main interests of the group is spectroscopy of organic molecules. I have studied organic systems like stilbene, stilbenoid molecules and azobenzene with quantum chemical methods, to determine the structure, reactivity and electronic spectra of such systems. [30], [31], [33], [42], [44].

I have also continued to work in my main area of research, i.e. quantum chemistry for heavy element systems. I have studied uranyl and neptunyl carbonate complexes in solution. The redox reaction of U(VI) to U(V) has been investigated together with the explicit bonding to water molecules in solution [23], [28]. I have studied the spectroscopy of small actinide systems like UO_2 in the gas phase [27], [34], [36]-[39].

In 2002 I have started to explore a new area of compounds formed by nitrogen clusters and metal atoms, such as actinides, lanthanides or transition metals. The idea that I have started to investigate is that nitrogen clusters [15], [16], [25], which are metastable compounds, could be stabilized by the presence of a metal with high angular momentum orbitals able to form bonds. This seems to be an innovative idea investigated for the first time by me, in collaboration with Professor Pekka Pykkö [26], [29], [32], [35], [39]. This work has been cited and highlighted in articles in Chemical and Engineering News (Vol 79 n. 40 p.24 Oct 01 2001) and Nature (Nature Science Update Sept. 17 2002).

Since then I have been working with the idea of predicting new chemical species containing metals. The behavior of gold as a halogen has been discovered [40], [47], and some short metal-metal bonds have been predicted [41]. Some of the predicted species have been recently synthesised by experimental groups. Professor Karl Cristhe has made some Ti tetrazides (Angew. Chem. vol 43, 3148 (2004)) and Professor Lai-Sheng Wang has made $TiAu_4$ and related species (Angew. Chem. vol 43, 2125 (2004)).

Recently I have also been studying some mixed metal-hydrogen compounds with general formula MH_{12}, where M=Cr, Mo, W [48]. They have interesting properties related to the hydrogen storage problem.

In July 2004 I was awarded the annual prize of the International Academy in Quantum Molecular Science (http://www.iaqms.org/IAQMS.awards.html) with the following citation:

”for her innovative contributions to prediction and understanding of new inorganic molecules using quantum chemical methods”

Thanks to my experience on DFT methods acquired in Cambridge, I have contributed to the implementation of a DFT module in the MOLCAS quantum chemistry package in collaboration with the Lund group. I have also started developing combined quantum chemistry and statistical mechanics approaches in order to study heavy element chemistry is solution. The quantum chemical side is based on accurate calculations of molecular properties in ground and excited states of molecules in solution. The solvent effects effects are taken into account dynamically. The method could be based on the NEMO model, which has been developed by Professor Gunnar Karlström and his collaborators in Lund. The approach has hitherto mainly been used for weak interactions between neutral molecules. Here I wish to extend the scheme to strongly interacting multi-charged ions with solute molecules [46].

In the fall of 2003 and in August 2004, I have been visiting Professor at the University of Tokyo. I have collaborated with Professor Hirao’s group on some projects on heavy element chemistry, with special focus on the chemiionization reactions of SmO [44] and UO [50].

I have now one Ph.D. student, Francesco Ferrante and one undergraduate student, Remedios Cortese.

3 Teaching

1997-1998: In Cambridge I have supervised some students within the course 'Introduction to Quantum Mechanics' by Dr. A.J. Stone.

1999-2000: I gave two lectures on 'Quantum chemistry and heavy element systems', at the School of Computational Chemistry organized by Professor V. Barone, Perugia, August 2000.

I was exercise leader at the European Summer School in Quantum Chemistry, Riolo Terme, Italy, September 2000.

2001: I gave a ten hour course on 'Group theory in chemistry' for undergraduates at the Department of Chemistry G. Ciamician, Bologna University.

I was exercise leader at the European Summer School in Quantum Chemistry, Tjörnap, August 2001, Sweden.

October-December 2002 50 hour course in Principle of Quantum Mechanics to 3rd year Chemistry students, Palermo University.

March-June 2004 50 hour course in Molecular Spectroscopy to 4th year Chemistry students, Palermo University.

4 International Schools and Conferences

1995: ”European Summer School in Quantum Chemistry”, Lund, Sweden.

1996: ”Fourth Summer School in Quantum Chemistry” Aarhus, Denmark.

September 1996: ”International Conference on Molecular Properties ”, Strasbourg, France, oral communication.

June 1997: ”Symposium on Density Functional Theory and applications”, Duke University, USA, poster.

June 1997: ”IX International Conference in Quantum Chemistry”, Atlanta, USA, poster.

May 1998: ”REHE Workshop: Theoretical tools for lanthanides and actinides chemistry”, Aspect, France, poster.

March 1999: ”Meeting of the American Physical Society”, Atlanta USA, oral communication.

April 1999: ”Relativistic Effects in heavy-Element Chemistry and Physics”, Maratea, Italy, poster.

September 1999: ”IXth International Density Functional Conference”, Roma, Italy, oral communication.

June 2000: ”Very Heavy Metals 2000” (satellite symposium of the Xth International Congress of Quantum Chemistry), Presqu’ile de Giens, Francia, invited lecture *Spin-orbit coupling in DFT* .

June 2000: ”Xth International Congress of Quantum Chemistry”, Mentone, France, poster.

April 2001: ”Relativistic Effects in heavy-Element Chemistry and Physics”, Kerkrade, The Netherlands, invited lecture *Actinide chemistry: the CASSCF/CASPT2 approach*.

July 2001: ”Molecular Quantum Mechanics: The right answer for the right reason”, Seattle, USA, poster.

July 2002: ”American Conference on Theoretical Chemistry Champion, Pennsylvania, USA, poster.

August 2002: ”WATOC 2002” Lugano, oral communication.

September 2002: ”12th European Seminar on Computational Methods in Quantum Chemistry”, Utrecht, The Netherlands, invited lecture *Recent advances in actinide chemistry*.

April 2003: ”Faraday Discussion: Quantum Inorganic Chemistry”, York, UK, oral communication.

July 2003: ”International Conference in Quantum Chemistry”, Bonn, Germany, poster.

February 2004: ”Theory and Applications of Computational Chemistry”, Gyeongju, Korea, oral communication.

July 2004: ”36 International Conference on Coordination Chemistry”, Merida, Mexico, oral communication.

July 2004: ”Molecular Quantum Mechanics, conference in honor of Nicholas Handy”, Cambridge, UK, poster.

5 List of Publications

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Full configuration interaction calculations on Be_2
Chem. Phys., **5**, 47 (1994)

[4] S. Evangelisti G.L. Bendazzoli and L. Gagliardi
Complete Active Space Configuration Interaction calculations with optimized orbitals: application to Li_2
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[5] S. Evangelisti and L. Gagliardi
A Complete Active-Space Self-Consistent-Field Study on Cubic N_8
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Direct-List Algorithm for Configuration Interaction Calculations
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[8] L. Gagliardi, S. Evangelisti P.O. Widmark and B.O. Roos
A Theoretical Study of the N_8 Cubane to N_8 Pentalene Isomerization Reaction
Theor. Chem. Accounts, **7**, 136 (1998)

[9] L. Gagliardi, S. Evangelisti, B.O. Roos and P.O. Widmark

A Theoretical Study of Ten N_8 Isomers

Theochem-J. Mol. Struct. **8**, 1 (1998)

[10] L. Gagliardi, N. C. Handy, A. G. Ioannou, C.-K. Skylaris, S. Spencer, A. Willetts and A. Simper

A two-centre implementation of the Douglas-Kroll transformation in relativistic calculations

Chem. Phys. Lett. **283**, 187193 (1998)

[11] L. Gagliardi, A. Willetts, C.-K. Skylaris, N. C. Handy, S. Spencer, A. G. Ioannou and A. M. Simper

A relativistic density functional study on the uranium hexafluoride and plutonium hexafluoride monomer and dimer species

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The hydration of UO_2^{2+} and PuO_2^{2+}

J. Phys. Chem. A **103**, 1831 (1999)

[14] L. Gagliardi, N. C. Handy, C.-K. Skylaris, and A. Willetts

A theoretical study on some Plutonium diketones

Chem. Phys., **252**, 47 (2000)

[15] L. Gagliardi, S. Evangelisti, A. Bernhardsson, R. Lindh and B.O. Roos

Dissociation reaction of N_8 azapentalene to 4 N_2: a theoretical study

Int. J. Q. Chem., **77**, 311 (2000)

[16] L. Gagliardi, S. Evangelisti, V. Barone, and B.O. Roos

On the dissociation of N_6 into 3 N_2 molecules

Chem. Phys. Lett., **320**, 518 (2000)

[17] C.-K. Skylaris, L. Gagliardi, N. C. Handy, A. G. Ioannou, S. Spencer A. Willetts and A. M. Simper

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A density functional study of plutonyl trifluoroacetone complexes in the gas phase and in solution

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[21] L. Gagliardi and B. O. Roos

Uranium triatomic compounds XUY (X,Y=C,N,O): a combined multiconfigurational second order perturbation and density functional study

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Theor. Chem. Acc. **106** 178-187 (2001)

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On the formation of pure nitrogen salts from N_3^-, N_5^+ and N_5^-

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J. Am. Chem. Soc., **124**, 8757-8761 (2002)

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Faraday Discussion, **124**, 63-68 (2003)

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