GIUSEPPE MALLIA

Date of birth: 04/06/1975 Nationality: Italian

ACADEMIC

1994-1999 ***Degree on Materials Science*** at University of Turin. Award: 16/12/1999
Supervisor: Prof. R. Dovesi, Theoretical Chemistry Group, University of Turin
Thesis: *Studio quanto meccanico di difetti paramagnetici in solidi ionici. (Quantum mechanical study of paramagnetic defects in ionic solids.)*

2000-2002 ***PhD in Material Science and Technology***, Faculty of Science-University of Turin
Supervisor: Prof. R. Dovesi, Theoretical Chemistry Group, University of Turin
Thesis: *Tecniche quanto-meccaniche ab initio per lo studio di proprietà elettroniche nei solidi. (Quantum mechanical ab initio techniques for the study of electronic properties in solids.)* Written in English. Award: 10/4/2003

2/1/2003-31/3/2003
grant for "Quantum mechanical methods for the study of dielectric properties in crystalline solids", at Dipartimento di Chimica I.F.M. of Turin
(Borsa di Studio per Addestramento alla Ricerca)

01/04/2003-30/04/2004
Post-doc position inside the EU funded "NUCLEUS" project
at Davy Faraday Research Laboratory in the Royal Institution of Great Britain.
Supervisor: Prof. A. R. C. Catlow
(15/6/2003-25/6/2003 research period at AMOLF, the Institute for Atomic and Molecular Physics in Amsterdam, under the supervision of Prof. Daan Frenkel)

01/05/2004 - **PRESENT POSITION**
Post-doc position at the Chemistry Department of Imperial College of London
Supervisor: Prof. N. M. Harrison

RESEARCH ACTIVITY AND SCIENTIFIC INTERESTS

My main research activity has involved the development and application of first-principles electronic structure calculation techniques. In particular, I have extensive experience in the use of the **CRYSTAL** package. This code is developed by the Computational Chemistry Group of the University of Turin, together with the Computational Materials Science Group of the Daresbury Laboratory. During the time spent in Turin's Group, I had the chance to acquire knowledge in the structure of CRYSTAL code and to help in its developments. *My contribution concerns the subroutines for the calculation of the optical dielectric constants* based on a macroscopic average of the electron density and of the electric field in the material by mean of supercell scheme.
At the Imperial College, I have the opportunity to extend my experience to the massive parallel (MPP) version of the program and I help in testing/documenting the MPP version.

In what concerns to the application of the techniques, my research has been focused on the following systems and properties:

CHEMICAL PROPERTIES

1) **Surfaces**: non-polar low indices surfaces of α-Al_2O_3. Slab approach. Surface formation energy. Relaxation effects. Electrostatic potential. Reactivity.

2) **Adsoption**: TiO_2. Slab thickness. CH_2CHF adsorption at rutile (110). Coverage effects. Total charge density maps. Density of states. Vibrational frequencies of adsorbate.

ELECTRIC PROPERTIES

3) Effect of an **electric field** and **dielectric constant** in ionic solid (LiF, MgO and BeO) and covalent/ionic crystal ($CaSO_4$). Refraction index. Dielectric tensor. Study of the band structure and of the band gap as a function of the applied field. Dielectric breakdown.

MAGNETIC PROPERTIES

4) **Point defects in crystals**: F center in alkali halides, trapped hole center in alkaline earth oxides. Supercell approach. Defect formation energy and relaxation effects. Paramagnetic defects. Spin Hamiltonian. Spin density maps. Band structure of the defective systems. Hyperfine interaction, isotropic (Fermi contact) and anisotropic coupling constants.

5) **Transition metal oxides in various magnetic states**: ferromagnetic FM, anti-ferromagnetic AFM of $KMnF_3$ and NiO. Open shell formalism. Ising Hamiltonian. The FM-AFM energy difference. Magnetic exchange coupling constant J. Superexchange. Spin density maps.

6) **Oxide based Dilute Magnetic Semiconductor (DMS) in Spintronics**: Transition metal-doped TiO_2. Substitutional and vacancy doping. Impurity oxidation state. Dilute regime: supercell approach. Room temperature ferromagnetism. FM and AFM phases. Fock exchange effects. Wannier functions. Density of states.

Experience in the use of 1) quantum mechanical code: Gaussian, Dmol
2) interatomic potential programs: GULP, DL_POLY

PUBLICATIONS

8) G. Mallia and N.M. Harrison
Magnetic moment and coupling mechanism of iron-doped rutile TiO_2 from first principles
Phys. Rev. B, 75, 165201 (2007)

7) G. Mallia, R. Dovesi and F. Corà
The anisotropy of dielectric properties in the orthorhombic and hexagonal structures of Anhydrite. An ab initio and hybrid DFT study
phys. stat. sol. (b), 243, 2935 (2006), 10.1002/pssb.200642161

6) J. Scaranto, G. Mallia, S. Giorgianni, C.M. Zicovich-Wilson, B. Civalleri, N.M. Harrison
A quantum-mechanical study of the vinyl fluoride adsorbed on the rutile TiO_2(110) surface, Surface Science 600 (2): 305-317 Jan 15 2006

5) F. Corà, M. Alfredsson, G. Mallia, D.S. Middlemiss, W.C. Mackrodt, R. Dovesi and R. Orlando, *The Performance of Hybrid Density Functionals in Solid State Chemistry*

in J. McGrady and N. Kaltsoyannis (Ed.),
Density Functional Theory in Inorganic Chemistry, Structure and Bonding, 113, 171-232, Springer-Verlag, Heidelberg, (2004).

4) C. Darrigan, M. Rérat, G. Mallia, R. Dovesi
Implementation of the finite field perturbation method in the CRYSTAL program for calculating the dielectric constant of periodic systems
J. Comput. Chem., 24, 11, 1305-1312 (2003)

3) G. Mallia, R. Orlando, M. Llunell, R. Dovesi
On the performance of various Hamiltonians in the study of crystalline compounds. The case of open shell systems, Computational Materials Science
C. R. A. Catlow and E.A. Kotomin (Eds.), IOS Press, 2003, 102-121

2) G. Mallia, R. Orlando, C. Roetti, P. Ugliengo, R. Dovesi
F center in LiF: a quantum mechanical ab initio investigation of the hyperfine interaction between the unpaired electron and the vacancy and its first seven neighbors
Phys. Rev. B, 63, 235102 (2001)

1) A. Lichanot, R. Orlando, G. Mallia, M. Merawa and R. Dovesi
V_{OH} center in magnesium oxide: an ab initio supercell study
Chem. Phys. Lett. 318, 240 (2000)

INVITED TALK

2) "Implementation of the high frequency dielectric constant for periodic systems in the CRYSTAL code.", presented at "Seminars for the PhD in Material Science", Directed by Prof. G.P. Brivio, Milan, Italy, 19 April 2004

1) "On the relative stability of various surfaces of α-Al_2O_3. An *ab initio* study" presented at Advanced School on Nanostructured Interfaces and Interphases Directed by Prof. D. Scarano, Torino, Italy, 1-3 September 2002

POSTERS

5) "*Magnetic moment and coupling mechanism of iron-doped TiO_2 from first principles."* presented at Davy Faraday Research Laboratory Day Annual Meeting 26 March 2007

4) "*A periodic quantum-mechanical study of Iron-doped Rutile TiO_2*" presented at "MSSC2006 - Ab initio Modelling in Solid State Chemistry" Directed by Prof. R. Dovesi, Torino, Italy, 3-8 Sep 2006

3) "The anisotropy of dielectric properties in the hexagonal and orthorhombic structures of Anhydrite. An *ab initio* quantum-mechanical study." presented at "LCC2004 - Local correlation methods: From molecules to crystals" Directed by Prof. C. Pisani and Prof. R. Dovesi, Turin Italy 9-11 Sep 2004

2) "Computational study of the interaction between Zn^{2+} and S^{2-} in the presence of water" presented at Davy Faraday Research Laboratory Day, 23 March 2004

1) "On the relative stability of various surfaces of α-Al_2O_3. An *ab initio* study"
presented at Euresco Conference on "Fundamental Aspects of Surface Science - Structure and reactivity of oxide surfaces"
Directed by Prof. G. Pacchioni, Acquafredda di Maratea, Italy, 1-6 June 2002

TEACHING AND SUPERVISING EXPERIENCE

9/7/2007-10/10/2007

Co-supervision of a UROP (University Research Opportunity Programme) student Mr Lee Kihong (Korea Science Academy Student)
Title of the project:"The computational modelling of novel fluorination catalyst"

12/2/2007-23/2/2007 SPRING TERM

3rd year Undergraduate - Chemistry - Computational Laboratory
Module: "Quantum-mechanical simulation of the electronic structure in solids"
In this module, students use a quantum-mechanical program (CRYSTAL) to calculate the electronic properties of an ionic, a covalent, a molecular and a metallic crystal.

12/2/2007-16/2/2007, 5/3/2007-9/3/2007 SPRING TERM

2nd year Undergraduate - Chemistry - Computational Laboratory
Module: "The Free Energy and Thermal Expansion of MgO"

5/2/2007-9/2/2007, 26/2/2007-2/3/2007 SPRING TERM

2nd year Undergraduate - Chemistry - Computational Laboratory
Module: "An exciting journey in the electronic structures"

30/1/2007-1/2/2007, 20/2/2007-22/2/2007 SPRING TERM

2nd year Undergraduate - Chemistry – Problem Class
Theoretical methods in chemistry: sequences, series, Morse potential, harmonic approximation, vibrational modes

7/11/2006, 5/12/2006 AUTUMN TERM

2nd year Undergraduate - Chemistry – Problem Class
Theoretical methods in chemistry: LCAO Theory of Ethene and Butadiene

3/9/2006-8/9/2006

responsible of tutorial sessions in the European Summerschool "MSSC2006 - Ab initio Modelling in Solid State Chemistry"
Directed by Prof. R. Dovesi, Torino, Italy

26/6/2006-8/9/2006

Co-supervision of a UROP (University Research Opportunity Programme) student Mr K. Dingle (Imperial College)
Title of the project: "Ferromagnetism in Fe-doped NiO"

13/2/2006-24/2/2006 SPRING TERM

3rd year Undergraduate - Chemistry - Computational Laboratory
Module: "Quantum-mechanical simulation of the electronic structure in solids"

In this module, students use a quantum-mechanical program (CRYSTAL) to calculate the electronic properties of an ionic, a covalent, a molecular and a metallic crystal.

6/2/2006-10/2/2006, 27/2/2006-3/3/2006 SPRING TERM
2nd year Undergraduate - Chemistry - Computational Laboratory
Module: "The Free Energy and Thermal Expansion of MgO"

31/1/2006-2/2/2006, 21/2/2006-23/2/2006 SPRING TERM
2nd year Undergraduate - Chemistry – Problem Class
Theoretical methods in chemistry: sequences, series, Morse potential, harmonic approximation, vibrational modes

20/9/2004-24/9/2004
responsible of tutorial sessions in the European Summerschool
"MSSC2004 - Modeling in Solid State Chemistry",
Directed by Prof. N.M. Harrison, Prof. R. Dovesi, Dr. F. Cora' , London, UK

15/11/2004-19/11/2004, 13/12/2004-17/12/2004 AUTUMN TERM
2nd year Undergraduate - Chemistry - Computational Laboratory
Module: The Free Energy and Thermal Expansion of MgO

2/11/2004-4/11/2004, 30/11/2004-2/12/2004 AUTUMN TERM
2nd year Undergraduate - Chemistry – Problem Class
Theoretical methods in chemistry: sequences, series, Morse potential, harmonic approximation, vibrational modes

7/9/2003-12/9/2003
responsible of the tutorial "Defects: vacancies, F-center and paramagnetic defects" in the European Summerschool
"MSSC2003 - Ab initio Modelling in Solid State Chemistry"
Directed by Prof. R. Dovesi, Torino, Italy

8/9/2002-13/9/2002
responsible of the tutorial "Defects: vacancies, F-center and paramagnetic defects" in the European Summerschool
"MSSC2002 - Ab initio Modelling in Solid State Chemistry"
Directed by Prof. R. Dovesi Torino, Italy

11/9/2001-15/9/2001
responsible of the tutorial "Defects: vacancies, F-center and paramagnetic defects" in the European Summerschool
"MSSC2001 - Ab initio Modelling in Solid State Chemistry"
Directed by Prof. R. Dovesi Torino, Italy

1998/1999 grant for part-time collaboration activity (50 hours)
for the "Material Laboratory" (I module)

1997/1998 grant for part-time collaboration activity (100 hours)
for the "Calculus and Programming Laboratory" (I-II modules)

EXPERIENCE ON COMPUTER SYSTEMS

Operating Systems: Unix/Linux, Windows 95/98/XP
Platforms: Intel based Platforms (serial, cluster, parallel)
DEC/Alpha, SUN/Sparc, IBM, HP Workstations (serial, parallel)
Programming Languages: FORTRAN90, MPI(mpich/lam), Shells,
makefile, cvs, matlab, HTML, perl (basic knowledge)

2000-2002 responsible of the Linux Intel PC and Sun Workstations
(OS installation and maintenance)
01/05/2004-NOW responsible of the PCs of the group (OS installation and maintenance)

ADDITIONAL FORMATION ON RELATED SUBJECTS

A*) MATERIAL SCIENCE

A1) Second Summer School on Computational Chemistry
Directed by Prof. P. Fantucci, Milano, Italy 24-28 July 2000

A2) European Summerschool "Ab initio Modelling in Solid State Chemistry"
Directed by Prof. R. Dovesi, Torino, Italy, 16-20 September 2000

A3) International Workshop on Characterization and Reactivity of
Surface Structures and Surface Species
Directed by Prof. A. Zecchina, Prof. C. Morterra, Prof. S. Coluccia
Torino, Italy 12-13 January 2001

A4) Euresco Conference on "Fundamental Aspects of Surface Science -
Structure and reactivity of oxide surfaces"
Directed by Prof. G. Pacchioni, Acquafredda di Maratea, Italy, 1-6 June 2002

A5) Advanced School on Nanostructured Interfaces and Interphases
Directed by Prof. D. Scarano, Torino, Italy, 1-3 September 2002

A6) EU funded "NUCLEUS" project meeting
Directed by Prof. J. Rosenholm, Turku, Finland, 26-27 September 2003

A7) "LCC2004 - Local correlation methods: From molecules to crystals"
Directed by Prof. C. Pisani and Prof. R. Dovesi, Turin Italy 9-11 Sep 2004

A8) "NIS Colloquium – Ab initio simulation of the properties of the Cristalline
Surfaces and Interfaces: Progress and Prospects",
Directed by Prof. A. Zecchina, Turin, Italy, 19-20 May 2005

A9) "Understanding and Prediction of Magnetic Properties in Molecules and
Solids", Directed by Prof. N. M. Harrison, London, 1-3 September 2005

A10) "Topics in Nano-Magnetism", Daresbury, UK (30 November 2005)

Organised by Prof W. Temmerman, Dr W. Hofer, Dr A. Wander and Prof N. Harrison

A11) "CRIM06: Current research in magnetism 2006", London, UK (18 December 2006)
Organised by Dr Oleg Petracic, Institute of Physics and Imperial College London

B*) PROGRAMMING

B1) "Introduction to FORTRAN 90"
Directed by Dr. G. Erbacci, Cineca, Bologna, Italy, 4-5 May 2000

B2) "FORTRAN 90 for intensive scientific calculation"
Directed by Dr. G. Bottoni, Cilea - Milano, Italy, 7-9 November 2000

C*) TEACHING

C1) "Learning for teaching", by Prof. F. Harrison, IC-London, 9-10 Dec. 2004

LANGUAGES

Italian: Mother Language
English: Certificate in Advanced English, Cambridge University, June 2005

HOBBIES

swimming, running, volley, dancing, reading, chatting with unknown people.

RECOGNITIONS

1) 'Optime' price by the Unione Industriale di Torino, reserved to the best graduated students in Torino for the AA 1998-1999

2) Medal for Best Thesis in Material Science in 1998/1999