

### *Personal Informations*

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- **Nationality:** Italian
- **Date of birth:** 25/08/1970

### *Education and Training*

- **1997:** Degree *summa cum laude* in chemistry under Prof. F. A. Gianturco at University “La Sapienza”, Rome (IT). Dissertation title: “computation of Exchange forces in molecule-electron collision processes”
- **2000:** PhD in chemistry under Prof. R. Caminiti at University “La Sapienza”, Rome (IT). Dissertation title: “Structures and processes in solid phase studied by mean of molecular dynamics and X-ray diffraction”

### *Working Experience*

- **1994-1995, 1995-1996:** undergraduate lab assistant at University “La Sapienza” for the course “Physical Chemistry”. In this context he taught: i) group theory for quantum mechanics, ii) theoretical spectroscopy, iii) X-ray diffraction theory and iv) Fortran programming
- **1999-2000:** visiting research fellow of the group of Prof. Michele Parrinello, Max-Plank institut fuer Festkoerperforchung, Stuttgart (GE)
- **2001:** visiting research fellow of the group of Prof. Roberto Car, Dept. Of Chemistry, Princeton University, Princeton (NJ, US)
- **2001:** Research Fellow of CASPUR, Inter-University Consortium for the Application of Super-Computing for Universities and Research
- **2002-** : staff member of CASPUR SuperComputing Centre
- **2003-** : team leader of two scientific software projects: CMSapi and CMPTool. CMSapi is a library of routines for atomistic simulations. CMSapi implements several molecular dynamics (MD) and rare event sampling algorithms, classical and tight binding potentials and routines to calculate standard properties (kinetic energy, stress tensor, etc.). CMPTool is a complete program for atomistic molecular and rare event simulations of atomistic systems. CMPTool uses CMSapi as MD engine (see <https://cmsportal.caspur.it/index.php/CMPTool>)
- **2006-**: Project Officer of the European Science Foundation Forward Look “Computational Science Forum: the Lincei Initiative.” The aim of this ESF Forward Look is to design and an infrastructure for development, maintenance and support of scientific software at a European level. The aim of this ESF Forward Look is also to create the political conditions necessary to implement such an infrastructure. (see <http://cyberinfrastructure.caspur.it/index.php> and <http://www.esf.org/activities/forward->

[looks/physical-and-engineering-sciences-pesc/current-forward-looks-in-physical-and-engineering-sciences/european-computational-science-the-lincei-initiative-from-computers-to-scientific-excellence.html](http://looks/physical-and-engineering-sciences-pesc/current-forward-looks-in-physical-and-engineering-sciences/european-computational-science-the-lincei-initiative-from-computers-to-scientific-excellence.html)).

### *Teaching Experience*

- **2004-** : organiser and teacher of a series of courses on Scientific and Technical Computing at CASPUR
- **2005-** : teaching assistant of Prof. Ciccotti for the course “Atomistic and Molecular Simulations”, University “La Sapienza” and RomaTre, Roma (IT). DL\_POLY has been used for the lab sessions of the year 2007 course
- **2005-** : Teacher of the course “Parallel and vector Programming” at the CASPUR “Summer School on Advanced Computing” (see <http://www.caspur.it/attivitae SERVIZI/scuolaestiva/>, in Italian)
- **2007-** : organiser of the CASPUR HPC courses (see <http://CorsiHPC.caspur.it>, in Italian)

### *Programming skill*

- Expert on Fortran, C and mixed Fortran/C programming (for example, CMSapi library was designed to be linkable from both Fortran and C/C++). He is also an expert on parallel programming in MPI and OpenMP. CMPTool (see above) was parallelised adopting a 1D domain decomposition scheme using MPI. At EWOMP 2003, he gave a talk demonstrating how bad were the current implementations of reductions of arrays for molecular dynamics. He also proposed an alternative algorithm based on the BLAS routine DGEMV (see <http://www.rz.rwth-aachen.de/ewomp03/OMPtalks.html#Agenda>)
- Expert on all kinds of current general purpose computer architectures: scalar, vector, cluster and constellation. Dr. Simone Meloni started programming on a DEC Alpha serial machine and since then continued programming on all the modern architectures for scientific computing: IBM PWR2, PWR3, PWR4 and PWR5 parallel computers equipped with IBM High Performance switch, DEC/COMPAQ/HP Alpha equipped with ELAN interconnect, Intel PC and Itanium clusters equipped with Myrinet and Gigabit network, AMD Opteron clusters equipped with Infiniband interconnect, and NEC SX6 vector computer. Since 2002, He has been member of the teams that evaluated vector and parallel machines for the CASPUR consortium.
- Thanks to his knowledge of programming techniques and computer architectures, he proposed a reordering algorithm able to increase performance of MD simulations of a factor 2/3 (see “Efficient particle labelling in atomistic simulations”, J. Chem. Phys., 126 (2007), 121102). This method is also able to improve parallel performance of domain decomposition schemes making unnecessary the packing/unpacking step.

### *Research interests*

- Rare events. Dr. Simone Meloni is collaborating with Prof. Giovanni Ciccotti of University “La Sapienza” (Rome, Italy) on the study of hydrogenation/dehydrogenation processes in sodium alanates using sampling techniques recently proposed by Prof. Eric Vanden Eijnden of New York University (New York, US) (string method, temperature accelerated method, and single-sweep method; the latter, recently discussed in group seminar in Rome, has not yet been published).
- Dr. Simone Meloni, in collaboration with Prof. Luciano Colombo of University of Cagliari (Cagliari, Italy) is applying these methods to the problem of formation of silicon nano-crystal in

silicon rich silicon oxide matrices. These materials are promising for optoelectronics and solar cells.

- Dr. Simone Meloni is also continuing his collaboration with Prof. Roberto Car of the Princeton University and Dr. Amedeo Palma of CNR (Italy) on organic semi-conductors.

### *List of publications*

1. "Low-energy electron scattering from the water molecule: Angular distributions and rotational excitation", Gianturco FA, Meloni S, Paoletti P, Lucchese RR, Sanna NJ., Chem. Phys., 108 (1998), 4002-4012
2. "SO<sub>2</sub>Cl<sub>2</sub>, SOCl<sub>2</sub>: energy dispersive X-ray diffraction, ab initio and molecular dynamics calculation", Meloni S, Pieretti A, Bencivenni L, Albertini VR, Sadun C, Caminiti R, Comput. Mater. Sci., 20 (2001), 407-415
3. "The monoclinic I2 structure of bassanite, calcium sulphate hemihydrate (CaSO<sub>4</sub> – 0.5H<sub>2</sub>O)", Ballirano P, Maras A, Meloni S, Caminiti R, Eur. J. Mineral., 13 (2001), 985-993
4. "A novel implicit Newton-Raphson geometry optimization method for density functional theory calculations", Filippone F, Meloni S, Parrinello M, J. Chem. Phys., 115 (2001), 636-642
5. "Chemistry between magnesium and multiple molecules in tris(8-hydroxyquinoline) aluminum films", Meloni S, Palma A, Schwartz J, Kahn A, Car R, J. Am Chem. Soc., 125 (2003), 7808-7809
6. "Energy-dispersive X-ray diffraction on thin films and its application to superconducting samples", Albertini VR, Paci B, Meloni S, Caminiti R, Bencivenni L, J. Appl. Crystallogr., 36 (2003), 43-47
7. "Boron ripening in amorphous silicon by large scale molecular dynamics simulations", Mattoni A, Colombo L, Meloni S, Federico A, Rosati M, Comp. Mater. Sci., 30 (2004), 143-149,
8. "Computational Materials Science application programming interface (CMSapi): a tool for developing applications for atomistic simulations", Meloni S, Rosati M, Federico A, Ferraro L, Mattoni A, Colombo L, Comp. Phys. Comm., 169 (2005), 462-466
9. "Molecular and Solid State (8-hydroxy-quinoline)aluminum Interaction with Magnesium: a First Principles Study", Meloni S, Palma A, Kahn A, Schwartz J, Car R, J. Appl. Phys., 98 (2005), 023707
10. "Ab Initio Simulation of Carbon Clustering on an Ni(111) Surface: A Model of the Poisoning of Nickel-Based Catalysts", Kalibaeva G, Vuilleumier R, Meloni S, Alavi A, Ciccotti G, Rosei R, J. Phys. Chem. B, 110 (2006), 3638-3646
11. "Efficient particle labeling in atomistic simulations", Meloni S, Rosati M, Colombo L, J. Chem. Phys., 126 (2007), 121102
12. "Quasi-One-Dimensional K-O Chain in PTCDA Thin Films: Evidence from First-Principles Calculations", Zazza C, Meloni S, Palma A, Knupfer M, Fuentes GG, Car R, Phys. Rev. Lett., 98 (2007), 046401
13. "Dissociative versus molecular adsorption of phenol on Si(100) 2x1: a first principle calculation", Carbone M, Meloni S, Caminiti R, Phys. Rev. B, 76 (2007), 085332

### *Posters and oral presentations*

1. "SO<sub>2</sub>Cl<sub>2</sub>, SOCl<sub>2</sub>: Energy dispersive X-ray diffraction, ab-initio and molecular dynamics calculations", Advances In Computational Materials Science II, Italian-Swiss Workshop, S. Margherita di Pula, Cagliari (IT), 19-23 September 1997
2. "Theoretical Investigation of Magnesium-tris(8-hydroxyquinolino) Aluminum (ALq<sub>3</sub>) interface", The Workshop on Computational Material Science, 12th Edition, Villasimius (Sardinia, IT), 23-29 September 2002
3. "Interaction of Lead with Iron Clusters", Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms, 25 February – 1 March 2002 Kerkrade (NL)
4. "CMSPortal: A WEB User Interface to Computational Materials Science Applications", Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms, 25 February – 1 March 2002 Kerkrade (NL)
5. "Theoretical Investigation of Magnesium-tris(8-hydroxyquinolino) Aluminum (ALq<sub>3</sub>) interface", Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms, 25 February – 1 March 2002 Kerkrade (NL)
6. "Reduction on arrays: comparison of performances between different algorithms", Fifth European Workshop on OpenMP (EWOMP), 22-23 September 2003, Aachen (GE)
7. "Computational Material Science Application Programming Interface (CMSApi): a tool for developing applications for atomistic simulations", Conference on Computational Physics 2004, Genoa (IT) 01-04 September 2004
8. "Ab-initio study of carbon clustering on Ni(111) surface", Conference on Computational Physics 2004, Genoa (IT) 01-04 September 2004
9. "Computational Material Science Application Programming Interface (CMSApi): a tool for developing applications for atomistic simulations", INTERNATIONAL SCHOOL OF SOLID STATE PHYSICS - 34<sup>th</sup> course: Computer Simulations in Condensed Matter: from Materials to Chemical Biology.
10. "Hydrogen Diffusion in Sodium Alanates", Conference on Computational Physics 2007, Brussels (IT) 05-08 September 2007
11. "An ESF Forward Look for non-hardware aspects of Computational Science Infrastructure", Conference on Computational Physics 2007, Brussels (IT) 05-08 September 2007
12. "Ab-initio simulation of carbon clustering on Ni(111) surface: the bonding mechanism between Na and C.", Conference on Computational Physics 2007, Brussels (IT) 05-08 September 2007