

**CURRICULUM VITAE OF THE SCIENTIFIC ACTIVITY OF
SILVIA PICOZZI**

(L'Aquila, December 16th 2007)

- **Silvia Picozzi** (SP) was born in L'Aquila on **December, 5th, 1970**. She's **married** with **3 kids** (born in 1998, November 26th, 2000 April 27th and 2002, July 23rd).
- In September, 23rd 1994 she got her undergraduate degree in **Physics** at **University of L'Aquila** (mark **110/110 cum laude**), defending a theoretical thesis entitled "*Structural and electronic properties of superstructures of III-V semiconductors*" (advisor Prof. A. Continenza)
- She won a pre-doctoral fellowship from Istituto Nazionale di Fisica della Materia (**INFM**) at Dept. Of Physical Science, **Univ. Cagliari** with scientific advisor **Prof. Sandro Massidda**, focusing on "*First principles methods based on density functional theory: Applications to a CaF2 intralayer in a Si homojunction*", in collaboration with **Prof. Raffaele Resta**, Univ. Trieste (year 1995)
- November 1995: She started a **PhD program in Materials Science at Consorzio Camerino-L'Aquila-Perugia**.
- During the PhD program, she won a Grant from Italian Consiglio Nazionale delle ricerche (**CNR**) within the **SHORT TERM MOBILITY 1998** program (international exchange of young scientists) to spend a research period (summer 1998) at **Dept. of Physics and Astronomy, Northwestern University, Evanston, IL, USA**, in the group of **Prof. Arthur J. Freeman** (Project Title: "*First-principles corrections to the Local Density Approximation to the Density Functional Theory: "Model-GW" and "Screened exchange-LDA": Applications to III-V semiconductor alloys.*")
- December 18th 1998: she defended her PhD thesis entitled "*Potential barrier engineering at III-V semiconductor heterojunctions and nitrides/metal interfaces: an ab-initio all-electron study*" (advisor: **Prof. Alessandra Continenza**) and she obtains the title of Philosophiae Doctor in Material Science
- October 1998 - May 1999: she has been a consultant at **Quantum Materials Design, Inc. (USA)**.
- In the period 1-06-1999/31-05-2001 she had a post-doctoral fellowship ("Assegno di ricerca") from **University of L'Aquila**, in the group of **Prof. A. Continenza**, entitled "*Computational study of semiconductor interfaces (semiconductor/semiconductor, semiconductor/oxide, semiconductor/metal) to determine the potential discontinuity and the role of interface states - screened-exchange and model-GW calculations*"
- During the fellowship, she won a Grant from Italian Consiglio Nazionale delle ricerche (**CNR**) within the **SHORT TERM MOBILITY 1999** program (international exchange of young scientists) to spend a research period (summer 1999) at **Dept. of Physics and Astronomy, Northwestern University, Evanston, IL, USA**, in the group of **Prof. Arthur J. Freeman** (Project Title: "*Schottky barrier heights in nitride/metal systems*")
- During the fellowship, she has spent a research staying (Summer 2000) as "**visiting student**" at **Dept. of Physics and Astronomy, Northwestern University, Evanston, IL, USA**, in the group of **Prof. Arthur J. Freeman** (Project: "*Implementation of the Auger recombination and impact ionization in the FLAPW code*").

- In the period 1-06-2001/31-05-2003 she has been a research associate (“Assegno di ricerca”) of **INFN** at **Dept. Physics, Univ. L'Aquila**, in the group of **Prof. A. Continenza**, project title “*Magnetic semiconductors: ab-initio computational study of magnetic and electronic properties for bulk and interface systems*”
- She has won a **Grant from Fondazione “Angelo della Riccia”** to spend a research staying (Summer 2001) at **Dept. of Physics and Astronomy, Northwestern University, Evanston, IL, USA**, in the group of **Prof. Arthur J. Freeman** (Project title: “*Magnetic semiconductors: First principles calculations of structural, electronic and magnetic properties in bulk systems and interfaces*”)
- She has won a **Grant from Fondazione “Fulbright-Italia/USA”** to spend a research staying (Summer 2002) at **Dept. of Physics and Astronomy, Northwestern University, Evanston, IL, USA**, in the group of **Prof. Arthur J. Freeman** (not used for maternity leave)
- In the period 09-06-2003/14-12-2004 she has been a research associate (“ricercatore a tempo determinato”) of **INFN** in the group of Prof. A. Continenza on “*Electronic, magnetic and transport properties of materials for spintronics*”
- Since December 15th 2004 she has a **Tenure Track position** (“ricercatore a tempo determinato con tenure track”) at **INFN CNR** (regional Laboratory **CASTI** – Center for Scientific and Technological Assistance to Industries).
- During the research associate position, she won a Grant from Italian Consiglio Nazionale delle ricerche (**CNR**) within the **SHORT TERM MOBILITY 2004** program (international exchange of young scientists) to spend a research period (summer 2004) at **Forschungszentrum Juelich, Germania**, in the group of **Prof. Dr. Stefan Bluegel** (Project title: “*Non-collinear magnetism from first-principles*”)
- Grant from **DAAD – Deutsche Akademischer Austauschdienst** (B1 fellowship): summer 2006 at **Forschungszentrum Juelich, Germania**, in the group of **Prof. Dr. Stefan Bluegel**
- Silvia Picozzi is **referee** of prestigious journals (**Nature Materials, Physical Review Letters, Applied Physics Letters, Physical Review B**, Journal of Magnetism and Magnetic Materials, Journal of Physics and Chemistry of Solids, Physics Letters A).
- Member of the committee in the area “*Theory, Modelling and Materials Design*” of the **ICTMC-15** (International Conference on Ternary and Multinary compounds) conference.
- Conference co-chair with Prof. Dr. Stefan Bluegel (Forschungszentrum Juelich, Germany) and Prof. Laszlo Szunyogh (Univ. Budapest, Hungary, and CMS Vienna, Austria) of the **CompMag 2006 conference** (Computational Magnetism and Spintronics), funded by ESF and Forschungszentrum Juelich, held in Juelich (Oct. 2nd-4th 2006)
- **Scientific supervisor** of **Dr. Kunihiko Yamauchi** (Japan) who has a post-doc position (“Assegno di ricerca”) at **CASTI CNR-INFN Regional Lab**, since December 1st, 2006 on “*Computational Materials Design*” (Bando N. INFN AR 29/2006 del 1 Settembre 2006)
- Scientific coordinator of the scientific seminars in Condensed Matter Series regularly held at **CASTI**
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- Guest scientist at **Kavli Institute for Theoretical Physics, University of California Santa Barbara (USA)** in summer 2007, to take part to the research program “*Moments and Multiplets in Mott materials*” coordinated by Leon Balents, Matthew Fischer, Daniel Khomskii, George Sawatsky and Oleg Tchernyshyov.
- Project reviewer for United States Department of Energy (DOE).
- Evaluator for the European Community in the Seventh Framework Programme in 2007 (EC rules do not allow to disclose more details about the specific panel or call)
- Co-organizer of the interdisciplinary symposium „*Ferroc materials and novel functionalities*“ at the upcoming Deutsche Physicalische Gesellschaft meeting (to be held on 25-29 February 2008) in Berlin, along with Prof. I. Mertig, Dr. R. Pentcheva, Prof. W. Kleeman.
- Appointed as Member of the Examining Committee at the public defence of Björn Skubic’s doctoral thesis on September 21st, 2007 at Uppsala University, Sweden (thesis title: „*Spin dynamics and magnetic multilayers*“, supervisors Prof. Olle Eriksson and Prof. Lars Nordstroem)
- Appointed as Opponent of the Examining Committee at the public defence of Diana Iusan’s licentiate thesis on January 25th, 2008 at Uppsala University, Sweden (supervisors Prof. Olle Eriksson and Prof. Biplab Sanyal)
- Silvia Picozzi is coauthor of more about **80 publications** (most of which as first author) on international scientific journals, she has been invited to give seminars at many different scientific groups and meetings (see list below). Her knowledge of both spoken and written English is excellent and she can speak and understand good French.
- SP currently holds an Hirsch index factor of 14 (according to the ISI Web of Science) and her paper shave been cited more than 750 times.

II. SCIENTIFIC ACTIVITY

SP has a wide and long-standing experience with first-principles codes for the determination of the structural, electronic and magnetic properties (in particular with **FLAPW**, **DMol³**, **FLEUR** in addition to PWSCF, VASP and tight binding). The background of SP are within semiconductor physics (both “traditional” as well as “non-conventional” as diluted magnetic semiconductors and organic semiconductors), in terms of structural, electronic and transport properties. In the last few years, on the other hand, her main interests have been focused on magnetism and magnetic materials. This is evident from the research arguments briefly outlined below, listed in “chronological order”:

- **Semiconductor interfaces**

She has been involved with semiconductor/semiconductor and semiconductor/metal junctions, focusing on III-V semiconductors, ceramic materials (SiC) or nitrides. In this framework, the most relevant quantity – both from the fundamental as well as technological point of view - is the potential line-up; in particular, the effects of the interface geometry (in terms of bond lengths in proximity to the junction, chemical termination, growth direction, etc.) on the potential barrier and on the interface electronic states have been investigated. For some of the compounds, surface properties have been investigated, in presence and absence of a metal monolayer (i.e. GaN/Al).

- **Beyond Local Density Approximation: Screened Exchange**

It is well known that the density functional theory in the local density approximation does not accurately describe the excited state properties; in particular, energy band gaps in semiconductors are severely underestimated. Among the different schemes proposed to overcome these drawbacks, we recall Screened Exchange (sX-LDA), which includes a non-local potential using a Thomas-Fermi like screening. The sX-LDA method, implemented within FLAPW, gives an accurate description of conduction bands and effective masses in semiconductors and has been applied to binary and ternary compounds, surfaces and superlattices.

- **New materials for spintronics**

Within the promising field of spintronics (in which the electron spin, in addition to its charge, is exploited as an additional degree of freedom), SP has been involved in semiconducting systems with magnetic impurities and “concentrated” magnetic materials.

- The study has been focused on structural, electronic and magnetic properties of magnetic semiconductors:
 - a) MnX (X=P,As,Sb) compounds, as a function of the chemical components and crystal structure
 - b) Chalcopyrite structure of the II-Ge-V₂ (II = Cd, Zn e V = As, P) and Cu-III-VI₂ (III = Ga, Al e VI = S, Se) as a function of the spin configuration and Mn percentage.
 - c) Group IV (Si, Ge and SiGe alloys) doped with Mn, as a function of the spin configuration and Mn content; “digital alloys”, i.e. superstructures in which mono – or sub-monolayers of Mn are intercalated in a Ge matrix; competing phases, like Mn₅Ge₃, formed during the growth of MnGe diluted magnetic semiconductors when Mn exceeds a crytical content.
 - d) BeTe doped with Mn, Cr, V, as a function of the different magnetic impurity and following exchange mechanism.

For some of these materials, a ferromagnetic alignment was predicted, with related important consequences for spintronic applications.

- **Half-metals**

In this same framework, SP has studied half-metallic materials (i.e. carriers 100% spin-polarized, due to the metallic character and semiconducting for the up and down spin channels, respectively of the Heusler type (Co₂MnSi, Co₂MnGe, Co₂MnSn), with particular attention to the bulk properties (such as hyperfine fields, orbital and spin moments, magneto-optical properties such as kerr spectra and X-ray magnetic circular dichroism), interfaces with traditional semiconducting materials (such as Ge, GaAs) and defects (such as antisites, atomic swaps, etc.).

- **Auger recombination and Impact Ionization**

The Auger recombination process (and its inverse process, so called “Impact ionization”) have a particularly relevant role in the efficiency of semiconducting devices. SP has implemented in the FLAPW code a formalism (based on Fermi’s golden rule within sX-LDA density functional theory) in order to calculated Auger recombination rates (both for

holes and electrons) and/or impact ionization (both hole and electron initiated) in semiconductors. This formalism, applied to several different semiconductors (GaAs, InGaAs, InP, *etc.*) represents the first fully ab-initio calculation of the above mentioned rates. The obtained results show a satisfying agreement with available theory and experiment results, and suggest that this same approach might be applied to more complex materials, in order to predict recombination rates as a function of the carrier concentration, temperature, concentration, etc.

- **Organic Materials and nanotubes**

She focused on the physical mechanism at the basis of molecules on several different substrates. This activity is carried out in strong collaboration with the experimental group headed by Dr. Luca Ottaviano and Prof. Sandro Santucci at Dept. Physics, Univ. L'Aquila. The study is focused on the structural, electronic and transport properties of several different systems (such as carbon nanotubes and phthalocyanines) upon interaction with gases (such as NO₂, CO, O₃ *etc.*)

- **Multiferroics (*presently main research line*)**

Multiferroics are materials that show at the same time ferroelectricity and magnetic ordering. In particular, rare-earth manganites (such as TbMnO₃, HoMnO₃) show this behavior and the study is focused on understanding the link between the structural and magnetic properties, so as to highlight the delicate interplay between charge, spin and orbital ordering. We are mainly focusing on two categories:

1. *Bulk multiferroics*, such as orthorhombic distorted manganites (such as HoMnO₃ in the AFM-E spin configuration) where ferroelectricity was shown to occur due to a dual nature: a conventional “displacement” like mechanism and a purely electronic mechanism induced by the peculiar AFM-E spin-ordering
2. *Ferroelectric/ferromagnetic interfaces*: we are studying the [001] ordered interfaces between Co₂MnSi (a Heusler alloy with extremely high Curie temperature) and conventional ferroelectrics (such as BaTiO₃). The aim of the study is to highlight the effects of the magnetic (ferroelectric) alignment of the Heusler (oxide) material on BaTiO₃ (Co₂MnSi). The problem has also technological relevant implications, since it could be a candidate for the so-called “multiferroic tunnel junctions” or “four-state-devices”, in which the barrier of a conventional tunnel junction is made of a standard ferroelectric.

III. INVITED TALKS AT MEETINGS AND SCIENTIFIC GROUPS

In addition to a continuous activity at Dept. Physics, Univ. L'Aquila, SP has given the following talks:

1. Talk upon invitation from **Prof. A.J. Freeman** at **Northwestern University** entitled “*Schottky barrier heights at GaN/Al interfaces*”, August 17th 1998.
2. Talk upon invitation from **Prof. A.J. Freeman** at **Dept. of Physics and Astronomy, Northwestern University** entitled “*Structural and electronic properties of III-V ordered systems: beyond LDA*”, July 1999.
3. Talk upon invitation from **Prof. A.J. Freeman** at **Dept. of Physics and Astronomy, Northwestern University** entitled “*First steps towards the implementation of the Auger recombination coefficient using FLAPW*”, September 2000.

4. Talk upon invitation from **Prof. Paolo Lugli**, "*Impact ionization and Auger recombination in semiconductors*", March 21st 2001, at **Dip. Ing. Elettronica, Univ. Tor Vergata, Roma**.
5. "*Impact ionization in semiconductors: an ab-initio sX-LDA approach*", 27 July 2001, at **Dept. of Physics and Astronomy, California State University, Northridge, Ca, Usa**, upon invitation by **Prof. Ruqian Q. Wu**.
6. "*Impact ionization and Auger recombination in semiconductors: a first principles approach*", August 27th 2001, upon invitation of **Prof. Walter R.L. Lambrecht**, within the "Condensed Matter Seminars" at **Dept. of Physics and Astronomy, Case Western Reserve University, Cleveland, Ohio, Usa**
7. Talk upon invitation from **Prof. A.J. Freeman** at **Dept. of Physics and Astronomy, Northwestern University** entitled "*First principles detailed balance determination of Auger recombination and impact ionization rates in semiconductors*", September 7th 2001.
8. "*Potential barrier engineering at nitride/metal interfaces: an ab-initio study*", invited talk by **Prof. H. Luth** at **International Workshop on Nitride Semiconductors - IWN2002, Aachen, Germania** (22nd-25th July 2002).
9. "*Impact ionization rates and Auger recombination rates in semiconductors: Implementation within the sX-LDA FLAPW code*", invited talk by **Prof. S. Bluegel** at **FLAPW workshop, Juelich, Germania** (February 10th-11st 2003).
10. "*First-principles determination of Auger recombination and Impact Ionization rates in semiconductors*", Invited talk from the organizing committee (**A. Vulpiani, F. Dalfovo, L. Colombo, U. Marini Bettolo Marconi, G. Senatore**) at **XXII Convegno di Fisica Teorica e Struttura della Materia** (March 20-23 2003).
11. "*Accurate first principles detailed balance determination of Auger recombination and impact ionization rates in semiconductors*," talk upon invitation of **Prof. P. Lugli** at **International Workshop on Computational Electronics – IWCE9, Roma, Italia** (May 25-29 2003).
12. Talk upon invitation from **Prof. A.J. Freeman** at **Dept. of Physics and Astronomy, Northwestern University** entitled "*First principles calculations on ferromagnetic semiconductors*", July 15th 2003.
13. Talk invited by **Dr. Bernard Delley** at **Paul Scherrer Institut, Villigen, Switzerland** entitled "*First principles calculation of Auger recombination and Impact Ionization Rates in Semiconductors*", January 28th 2004.
14. Talk invited by **Prof. Dr. Stefan Bluegel** at **Forschungszentrum Juelich, Germany**, dal titolo "*First principles study of Heusler alloys for spintronic applications*", June 9th 2004.
15. Talk invited by **Dr. Arrigo Calzolari and Elisa Molinari** at **Dip. Fisica, Univ. Modena e Reggio Emilia, Italy** entitled "*Si-based spintronics: an overview on Mn-doped group IV semiconductors*" (November 23rd, 2004)
16. Talk invited by **Prof. M. Erbudak** at **ETH Zurich, Switzerland**, in the "Condensed Matter Seminar Series" entitled "*Si-based spintronics: an overview on Mn-doped group IV semiconductors*" (December 2nd, 2004)
17. Talk invited by **Prof. Dr. Stefan Bluegel** at **Forschungszentrum Juelich, Germany**, in the "Condensed Matter Seminar Series" entitled "*Si-based spintronics: an overview on Mn-doped group IV semiconductors*" (January 22th, 2005)
18. Talk invited by **Dr. Stefano Sanvito** at **Trinity College Dublin, Ireland**, entitled "*Si-based spintronics: an overview on Mn-doped group IV semiconductors*" (March 7th, 2005)
19. Invited talk at **AFOSSR Workshop on Wide Bandgap Ferromagnetic Semiconductors**, entitled "*First-principles approach to Mn-doped group IV semiconductors: examples and outlook*", Edinburgh, Scotland, May 15th.-19th 2005
20. Invited talk by **Prof. Franca Manghi** at **Dip. Fisica, Univ. Modena e Reggio Emilia, Italy** entitled "*First-principles approach to Heusler alloys for spintronic applications*" (June 7th, 2005)
21. Talk upon invitation from **Prof. A.J. Freeman** at **Dept. of Physics and Astronomy,**

- Northwestern University** entitled “*First-principles approach to Mn-doped group IV semiconductors: examples and outlook*”, June 20th 2005.
22. Nov. 23rd 2005: Invited talk by **Prof. Riccardo Bertacco, Politecnico di Milano, Italy** on “Towards Si-based spintronics: a first-principles overview on Mn-doped group IV semiconductors”
 23. Dec. 2nd 2005: Invited talk within the Condensed Matter Seminar Series at the **Johannes Gutenberg University, Mainz, Germany**, invited by **Prof. Claudia Felser** entitled “*First-principles approach to Heusler alloys for spintronic applications*”
 24. Dec. 12th-14th 2005: Invited talk suggested by the organizing committee (Profs. P. H. Dederichs and H. Katayama-Yoshida) at the **EU-JAPAN Workshop "Computational Nanomaterials Design"** held at CECAM, Lyon, France on “Towards Si-based spintronics: a first-principles overview on Mn-doped group IV semiconductors”
 25. March 6th 2006: Invited talk upon invitation of **Prof. Tamio Oguchi** held at Hiroshima Univ., Japan on “Towards Si-based spintronics: a first-principles overview on Mn-doped group IV semiconductors”
 26. March 7th-10th 2006: Invited talk suggested by the organizing committee (Profs. T. Matsumoto and T. Wada) at the “**International Conference on Ternary and Multinary compounds (ICTMC-15)**”, Kyoto, Japan on “First-principles calculations on magnetic semiconductors”.
 27. March 12th 2006: Invited talk upon invitation of **Prof. Hiroshi Katayama-Yoshida** held at ISIR (Institut for Scientific and Industrial Research, Osaka Univ., Japan) on “Towards Si-based spintronics: a first-principles overview on Mn-doped group IV semiconductors”
 28. March 9th 2007: Invited talk upon invitation of **Prof. Arthur J. Freeman** held at Northwestern University, Evanston, IL, USA on “Ferroelectric switching via spin rotations in orthorhombic distorted manganites”
 29. March 29th 2007: Invited talk in the magnetism division (head of Program Committee. **Prof. Dr. Eberhard Wassermann**) at the **Deutsche Physikalische Gesellschaft (DPG)** meeting in Regensburg, Germany (March 26th-30th 2007). Title of the talk: “First-principles study of ferromagnetic Heusler alloys: an overview”
 30. „*Dual nature of Improper ferroelectricity in a Magnetoelectric Multiferroic*“: Invited talk by the organizing committee (**M. Fischer, D. Khomskii, G. Sawatzky, N. Spaldin, O. Tchernyshyov**) at the „MOTTERIALS: spin, orbital and lattice physics near the Mott transition“ conference held in Santa Barbara, CA (Sept. 10th-14th 2007)

IV. FINANCED RESEARCH PROJECTS

SP has contributed to several different research projects:

1. Funded by **Universita' di L'Aquila** within the “**Support of Young investigators**” (2001): “*First principles calculations of the Auger recombination coefficient: implementation within the FLAPW code*”.
2. Project **INFN-Cineca: Iniziativa trasversale Calcolo Parallelo** su “*SSSS - Silicon/SuperSoft-Silicides interfaces: computational experiments*” (2001-2002).
3. Coworker in the project **PAIS-INFN Intersezione (D-E-F)** on “*Theoretical and experimental studies of magnetic properties MBE grown MnGe diluted magnetic semiconductor films*” (GEMASE), 2002-2003.
4. Coworker in the project **PRIN** of Italian Ministry of Research on “*Sviluppo di materiali nanostrutturati per sensori di gas selettivi ad altissima sensibilità per il monitoraggio di inquinanti atmosferici*”, 2002-2003.

5. Project **INFM-Cineca: Iniziativa trasversale Calcolo Parallelo** on “*Ab-initio study of gas sensing materials*” (2003).
6. **Project Manager of INFM-Cineca: Iniziativa trasversale Calcolo Parallelo** on “*Ab initio studies of surface structure of metal/silicon surface*” (2004).
7. **Barcelona Supercomputing center** (2006, third trimester) on “*Ab initio approach to multiferroics based on perovskites: exchange mechanisms and chemical trends*”
8. **Barcelona Supercomputing center** (2006, fourth trimester) on “*Ferroelectricity and magnetism in perovskite-like rare-earth manganites*”
9. **Barcelona Supercomputing center** (2007, first term) on “*Advanced multifunctional materials for spintronics*”
10. **Barcelona Supercomputing center** (2007, second term) on “*Spin meets ferroelectricity*”
11. **Barcelona Supercomputing center** (2007, third term) on “*Ferroelectricity and magnetism: coupling mechanism from ab-initio studies*”
12. Supercomputing grant at **Cineca 2007**: S. Picozzi, P. Monachesi, K. Yamauchi, B. Sanyal “*Spin meets ferroelectricity: ab-initio characterization and materials design for multiferroics*”, 35000 CPU hours

She is local-manager/hosting-supervisor for the following **international training projects**:

1) **INTAS Young Scientist Fellowship** Ref. Nr 05-109-4603 awarded to **Dr. Sergey Sarkisov**, Russian Academy of Sciences, Siberian Branch, Tomsk (Russia) to work on “*First principles study of transition-metal doped chalcopyrites for spintronic applications: characterization and design*” for two years (01-03-06/28-02-08)

2) International program for short-term research visits within the “**21st-Century Center of Excellence: Towards creating new industries based on Internanoscience**” di Osaka, Japan, awarded to **Dr. Kunihiko Yamauchi** from January 10th to February 20th 2006. Project title “*Electronic structure and material design for multiferroics using perovskite rare-earth manganites*”

3) International partial support by Natural National Science Foundation of China under Grant No. 10674027 to host for three months (Feb. 10th to May 10th 2006) **Dr. Chunlan Ma**, working on her PhD at University of Shanghai with Prof. Zhongqin Yang as PhD supervisor in China. Project title: “*First-principles approach to multiferroics based on rare-earth manganites*”

4) Consiglio Nazionale delle Ricerche - Deutsche Forschungsgemeinschaft (**CNR-DFG**) **cooperation program** between Italy and Germany to host **Dr. Marjana Lezaic**, Post-Doc in Forschungszentrum Juelich under the supervision of Prof. Dr. Stefan Bluegel, to work for three months in 2006 in L’Aquila. Project title: “*Exchange constants in diluted magnetic semiconductors: a first-principles study of their dependence on pressure and strain*”

5) International program for short-term research visits within the “**21st-Century Center of Excellence: Towards creating new industries based on Internanoscience**” di Osaka, Japan,

awarded to **Dr. Kunihiro Yamauchi** from August 25th to September 24th 2006. Project title “*Electronic structure and material design for multiferroics using perovskite rare-earth manganites (II)*”

5) CNR-Short Term Mobility program to host **Prof. Biplab Sanyal** (Uppsala Univ., Sweden) in 2006 to work on “*First principles approach to Multiferroics based on perovskites*” (in collaboration with Prof. Lucari)

In addition, she has hosted at CASTI the following scientists for scientific collaborations:

- **Dr. Phivos Mavropoulos**, Forschungszentrum Juelich, Germany (February 8th-10th 2006)
- **Dr. Bernard Delley**, Paul Scherrer Institut, Villigen, Switzerland (October 10th-13th 2006)
- **Dr. Kazunori Sato**, ISIR Osaka University, Japan (October 26th-28th 2006)
- **Dr. Lars Bergqvist**, Forschungszentrum Juelich, Germany (November 9th- December 9th 2006)
- **Prof. Tamio Oguchi**, Hiroshima University, Japan (March 11th-15th 2007)

V. MAIN SCIENTIFIC COLLABORATIONS

- **Prof. Elbio Dagotto**, Oak Ridge National Lab, TN, USA
- **Prof. Dr. Stefan Bluegel**, Forschungszentrum Juelich, Germany
- **Prof. Arthur J. Freeman**, Dept. of Phys. and Astronomy, Northwestern University, Evanston, IL, Usa

VI. ASSOCIATIONS

- American Physical Society (APS)

VIII. SUPERVISING EXPERIENCE

A. SP has co-supervised in their thesis works the following students:

Undergraduate/master students:

1. **Dr. Alessandro Stroppa**, “*Structural, Electronic and Magnetic properties of magnetic semiconductors*” (June 2002)
2. **Dr. Federica Di Gregorio**, “*Experimental and theoretical study on gas adsorption on carbon nanotubes*” (July 2003)
3. **Dr. Cinzia De Luca**, “*Ab-initio study of structural and electronic of polymer-nanotubes systems*” (July 2004)
4. **Dr. Elisa Liberatore**, “*Structural, electronic and magnetic properties of Mn-doped InAs, from first-principles*” (November 2003)
5. **Sig. Fabio Ricci**, “*First-principles magneto-optical studies on magnetic materials for spintronics*” (June 2006)

PhD Students of Dottorato in Fisica (XVII cycle):

1. **Dr. Mirko Simeoni**, “*Structural properties of systems based on organic materials: theory and experiments*” (March 2005)

Entitled to teach in high-school: “Abilitazione all'insegnamento di **matematica** (classe di concorso 47/a), **matematica e fisica** (classe di concorso 49/a) e **fisica** (classe 38/a), **vincitrice di concorso e titolare di cattedra** (prima di diventare dipendente del CNR-INFN e cioè prima del 09-06-2003) presso il liceo classico “M. Delfico” di Teramo”.