

Alessio Filippetti Curriculum Vitæ

Name: Alessio Filippetti

Place and Date of Birthday: Roma (Italy), 6 august 1966

Current Address: Department of Physics, University of Cagliari,
S.P. Monserrato-Sestu Km 0,700 I-09042 Monserrato (CA), ITALY
Tel.: (+39) (070) 675 4847, cell. phone: (+39) 348 9235909; Fax:
(+39) (070) 510171.
E-mail: alessio.filippetti@dsf.unica.it

Education and Job:

21/7/94: Achievement of Degree (Laurea) in Physics at the University of Rome "La Sapienza", Italy.

Thesis of Laurea entitled: "Chemical hardness and transferability of ionic pseudopotentials", with Professor Giovanni B. Bachelet.

08/1994-10/1994: Short-term visitor at Rutgers University, New Jersey, USA, to work in collaboration with Professor David Vanderbilt.

01/1995-01/1998: PhD student at the Physics Department of the University of Cagliari, Italy, supervised by Professors Vincenzo Fiorentini and Franco Meloni.

01/1998-12/1999: Researcher at the Physics Department of the University of California at Davis, in the group of Professors Warren E. Pickett and Barry M. Klein.

05/1998: PhD thesis discussion and official achievement of the PhD title at the University of Rome "Tor Vergata". Title of thesis: "Structural properties of Metallic and Semiconducting Surfaces".

12/1999-03/2003: Researcher at the Material Department of the University of California at Santa Barbara, in the group of Professor Nicola A. Spaldin.

03/2003-today: Visiting Professor at the Physics Department of the University of Cagliari, Italy, in the framework of project "Rientro Cervelli" supported by MIUR (Italian Ministry of University and Research)

Research interests and expertise:

Condensed matter physics: First-principles approach to the study of atoms and crystals. Main topics: surface and interface reconstructions, bulk and surface magnetism, ferroelectricity, multiferroics, high- T_c superconductors, doped Mott-Hubbard insulators and strongly-correlated compounds in general. Development and implementation of computational techniques.

Numerical simulations: Experience with code writing, numerical algorithms on serial and parallel computers (e.g. IBM SP2), UNIX, AVS, Mathematica.

Teaching

Year 2003-2004: lecturer of the class: “*Physics of Semiconductors*” (6 credits) for IVth year students of Physics degree (Laurea) at the University of Cagliari.

Year 2004-2005: lecturer of the class: “*Quantum theory of solids*” for students of the Ith year specialistic degree in Physics at the University of Cagliari.

Year 2005-2006: lecturer of the class: “*Magnetic properties of the matter*” (6 credits) for students of the 2nd year specialistic degree in physics, and “*Quantum theory of solids*” (6 credits) for students of the Ith year specialistic degree in physics at the University of Cagliari.

Year 2006-2007: lecturer of the class: “*Magnetic properties of the matter*” (6 credits) for students of the 2nd year specialistic degree in Physics, and “*Quantum theory of solids*” (6 credits) for students of the Ith year specialistic degree in Physics at the University of Cagliari.

List of Publications

1. **A. Filippetti**, D. Vanderbilt, W. Zhong, Y. Cai and G.B. Bachelet.
Chemical Hardness, Linear Response, and Pseudopotential Transferability.
Phys. Rev. B **52**, 11793 (1995).
2. **A. Filippetti**, V. Fiorentini, R. Valente, K. Stokbro and S. Baroni.
Formation energy, stress and relaxations of low-index rhodium surfaces.
in *Material theory, Simulations, and Parallel Algorithms*, edited by E. Kaxiras and J. D. Johannopoulos, MRS Proceedings **408**, 457-462 (1996).
3. V. Fiorentini, A. Bosin, S. Oppo, A. Satta, **A. Filippetti**, and D. Fois.
Ab-initio studies of material properties of wide-gap semiconductors, metal surfaces, and intermetallic alloys on vector and parallel supercomputers,
in *Sciences and Supercomputing*, edited by G. Erbacci and M. Voli (Cineca, Bologna 1996), p.527-534.
4. **A. Filippetti**, A. Satta, D. Vanderbilt and W. Zhong.
Hardness Conservation as a new transferability criterion: application to fully non-local pseudopotentials..
Int. J. Quant. Chem., **61** 3 (1997).
5. **A. Filippetti** and V. Fiorentini.
Reconstructions of Ir (110) and (100): an ab-initio study,
Surface Science, **377-379**, 112 (1997).
6. **A. Filippetti**, M. Menchi, A. Bosin, and G. Cappellini,
Relaxations at GaN (10 $\bar{1}$ 0) and (110) surfaces.
Proceedings of III-V Nitrides Symposium, MRS 1997 Fall Meeting.
7. **A. Filippetti**, V. Fiorentini, G. Cappellini and A. Bosin.
Ionicity and Relaxation Anomalies at III-V Nitride Surfaces,
Phys. Stat. Sol. (a) **170**, 265 (1998).

8. **A. Filippetti.**
Electron affinity in density-functional theory in the local-spin-density approximation,
Phys. Rev. A **57**, 914 (1998).
9. **A. Filippetti, V. Fiorentini, G. Cappellini and A. Bosin.**
Anomalous relaxations and chemical trends at III-V nitride non-polar surfaces,
Phys. Rev. B **59**, 8026 (1999).
10. **A. Filippetti and V. Fiorentini.**
Faceting and stress of missing-row reconstructed transition-metal (110) surfaces,
Phys. Rev. B **60**, 14366 (1999).
11. **A. Filippetti, W. E. Pickett and B. M. Klein,**
Competition between Magnetic and Structural Transitions in CrN,
Phys. Rev. B **59**, 7043 (1999).
12. **A. Filippetti and W. E. Pickett.**
Prediction of Ferromagnetic Ground State of NaCl-type FeN,
Phys. Rev. B **59**, 8397 (1999).
13. R. Weht, **A. Filippetti and W. E. Pickett,**
Electronic Characteristics of Quasi-2D Metalchloronitrides: Na_xHfNCl ($T_c=25$ K) Proceedings of HTS99 Conference, Miami (1999).
14. R. Weht, **A. Filippetti and W. E. Pickett,**
Electron doping in the honeycomb bilayer superconductors (Zr, Hf)NCl
Europhys. Lett. **48** (3), 320 (1999).
15. **A. Filippetti and W. E. Pickett**
Magnetic reconstruction at (001) CaMnO_3 surface.
Phys. Rev. Lett. **83**, 4184 (1999).
16. **A. Filippetti and V. Fiorentini.**
Theory and application of the stress density,
Phys. Rev. B. **61**, 8433 (2000).
17. **A. Filippetti and W. E. Pickett**
Double-exchange-driven spin pairing at the (001) surface of manganites.
Phys. Rev. B **62**, 11571 (2000).

18. **A. Filippetti** and Nicola A. Hill
Magnetic stress as a driving force of structural distortions: The case of CrN.
 Phys. Rev. Lett. **85**, 5166 (2000).
19. Nicola A. Hill and **A. Filippetti**
First principles study of two magnetic ferroelectrics
 Proceedings of the Pakistan Physical Society's 8th National Symposium on Frontiers in Physics, Government College, Lahore, Nov. 20-22 (2000).
20. **A. Filippetti** and V. Fiorentini.
Stress and reconstructions on (001) transition metal surfaces
 Comp. Mat. Sci. **20**, 423 (2001).
21. **A. Filippetti** and N. A. Hill
First Principles Study of structural, electronic and magnetic interplay in ferromagnetic yttrium manganite.
 Journal of Magnetism and Magn. Mat. **236**, 176 (2001).
22. **A. Filippetti** and Nicola A. Hill
On the coexistence of magnetism and ferroelectricity in perovskites.
 Phys. Rev. B, **65** (2002).
23. Nicola A. Hill and **A. Filippetti**
Why are there any magnetic ferroelectrics?
 Journal of Magnetism and Magn. Mat. **242-245**, 976 (2002).
24. **A. Filippetti** and Nicola A. Hill
A self-interaction corrected ultrasoft pseudopotential scheme for strongly-correlated and magnetic systems.
 Phys. Rev. B, **67**, 125109 (2003).
25. **A. Filippetti** and Nicola A. Spaldin
Strong-correlation effects in Born effective charges
 Phys. Rev. B, **68**, 045111 (2003).
26. B. Van Aken, T. M. Palstra, **A. Filippetti**, and N. A. Spaldin
The origin of ferroelectricity in magnetoelectric YMnO₃.
 Nature Materials, **3** 164 (2004).

27. **A. Filippetti**, N. A. Spaldin, and S. Sanvito
Self-interaction effects in (Ga,Mn)As and (Ga,Mn)N.
Chem. Phys., **309**, 59 (2005).
28. **A. Filippetti**, N. A. Spaldin, and S. Sanvito
Strong correlation and ferromagnetism in (Ga,Mn)As and (Ga,Mn)N.
Journal of Magnetism and Magn Mat., **290-291 P2**, 1391 (2005).
29. **A. Filippetti** and G. B. Bachelet
Electronic structure: the pseudopotential method.
in *Encyclopedia of Condensed Matter Physics*, Edited by Franco Bassani, Jerry Liedl, and Peter Wyder. (Elsevier, Netherlands).
(May 2005)
30. P. Delugas, V. Fiorentini, and **A. Filippetti**
Dielectric properties and long-wavelength optical modes of the high-k oxide LaAlO₃.
Phys. Rev. B, **71** 134302 (2005)
31. **A. Filippetti** and V. Fiorentini
Magnetic ordering in CuO from first-principles : a cuprate antiferromagnet with fully three-dimensional exchange interactions
Phys. Rev. Lett. **95**, 086405 (2005)
32. **A. Filippetti** and V. Fiorentini
Ionic and metal bonding in noble-metal cuprates
Phys. Rev. B, **72**, 035128 (2005)
33. C. Toher, **A. Filippetti**, S. Sanvito, Kieron Burke
Self-interaction errors in density-functional calculations of electronic transport
Phys. Rev. Lett. **95**, 146402 (2005)
34. P. Delugas, V. Fiorentini, and **A. Filippetti**
Dielectric properties of rare-earth oxides: general trends from theory
invited review in: Rare Earth Oxide Thin Films: Growth, Characterization and Applications, ed. M. Fanciulli and G. Scarel (Springer Topics in Applied Physics, Berlin 2006).
35. V. Fiorentini, P. Delugas, and **A. Filippetti**
A theoretical view on the dielectric properties crystalline and amorphous high- κ materials and films, invited review in Advanced Gate

Stacks on High-Mobility Semiconductors, ed. A. Dimoulas, E. Gusev, P. McIntyre, and M. Heyns (Springer, Berlin, 2006).

36. **A. Filippetti** and V. Fiorentini
Double-exchange driven metal-insulator transition in Mn-doped CuO
Submitted for publication
37. **A. Filippetti** and V. Fiorentini
Self-Interaction-free Density-Functional Band Theory for Magnetic Cuprates
J. Magnetism and Magn. Mat. (in print)
38. P. Delugas, V. Fiorentini, and **A. Filippetti**
First-principles calculations of high-k dielectric materials
invited review in: Multifunctional ceramic materials and films, Edited by L. Mitoseriu, Indian series of Appl. Phys.
39. **A. Filippetti** and V. Fiorentini
Magnetic ordering under strain and Spin-Pierls dimerization in GeCuO₃
Submitted for publication

Contributions to Conferences

1. **8/95, Paris:** *6th International Conference on the Applications of Density-Functional Theory to Chemistry and Physics.*
Poster contribution.
2. **12/95, Modena:** *Conference on Surfaces and Interfaces.*
Oral contribution.
3. **4/96, Stresa:** *Conference of European Physical Society.*
Poster contribution.
4. **9/96, Genova:** *European Conference on Surface Science (ECOSS 96).*
Poster contribution.
5. **10/96, S. Margherita di Pula (Cagliari):** *Italian-Swiss Workshop.*
Oral contribution.

6. **12/96, Boston:** *Fall 1996 Meeting of Material Research Society.*
Oral contribution.
7. **3/97, Fai della Paganella (Trento):** *16th Conference of Theoretical Physics and Condensed Matter Structure.*
Invited talk.
8. **4/97, Rome:** *Meeting of "Real atoms and solids, core and valence electrons" Network.*
Invited talk.
9. **6/97, Corfu:** *Euroconference on Total Energy Methods to study the Dynamics of surface process.*
Oral contribution
10. **3/98, Los Angeles:** *1998 March Meeting of American Physical Society.*
Oral contribution.
11. **5/98, Philadelphia:** *10th Annual Workshop on Recent Developments in Electronic Structure Algorithms (ES98).*
Poster contribution.
12. **3/99, Atlanta:** *1999 March Meeting of American Physical Society.*
Oral contribution.
13. **5/99, Urbana Champaign:** *New Methods in Electronic Structure Calculations.*
Poster contribution.
14. **8/99, Santa Barbara:** *Conference on Quantum Magnetism.*
Poster contribution.
15. **11/99, San Jose':** *Conference on Magnetism and Magnetic Materials.*
Oral contribution.
16. **3/00, Minneapolis:** *2000 March Meeting of American Physical Society.*
Two oral contributions.
17. **6/00, NIST (Gaithersburg, Md):** *Meeting of effective hamiltonian network.*
Oral contribution.

18. **2/01 Williamsburg:** *Ferroelectric workshop.*
Invited talk.
19. **3/01 Seattle:** *APS March Meeting.*
Oral contribution.
20. **9/01 Avignon:** *Workshop on thermodynamic and structural properties of materials.*
Invited talk.
21. **2/02 Washington:** *Physics of Ferroelectric.*
Invited talk.
22. **3/02, Indianapolis:** *2002 March Meeting of American Physical Society.*
Oral contribution.
23. **3/04, Montreal:** *2004 March Meeting of American Physical Society.*
Oral contribution.
24. **9/04, Geremeas:** *Workshop on Computational Material Science.*
Invited talk.
25. **3/05, Dublin:** *Trinity College, Physics. Dept..*
Invited lecture.
26. **4/05, Nagoya, Japan:** *INTERMAG 2005.*
poster presentation.
27. **6-10 6/05, Genova:** *COST school on ceramic materials.*
Invited lecture
28. **22-24 6/05, Genova:** *MMD-INFM meeting.*
Invited talk.
29. **20 feb 06, Trinity College Dublin**
Invited lecture
30. **12-18 mar 06, Baltimore:** March Meeting of American Physical Society.
Oral contributions (3).
31. **24 mar 06, Sestri Levante Satt13**
Oral contribution

32. **21 ago 06, Kyoto** International Conference on Magnetism 2006
Oral contribution
33. **21 sept 06, Palau** Material Modeling at nanoscale 2006
Chair of session: properties of strong-correlated materials.

Projects and proposals

- 1 **PRIN project** (research program of relevant national interest) funded by MIUR in december 2005 with 70,000 Euros for 2 years, entitled *Coexistence of magnetism and metallicity in high-Tc superconducting oxides* in collaboration with Vincenzo Fiorentini and Samuele Sanna.
- 1 **PRIN project** entitled *Realization and characterization of planar nanodevices based on colossal magnetoresistance materials* currently submitted, in collaboration with Physics Department of University of Genova, Italy.
- 1 **STREP project** (Specific targeted research project) submitted to the European Community, entitled *multiferroic thin film: from ceramics to heterostructures* in collaboration with groups from the following institutions: CNR of Genova (Italy), Academy of Science (Czech Republic), Forschungszentrum Julich (Germany), University of Aveiro (Portugal), Alexandru Ioan Cuza University (Romania), University of Stocholm, (Swe), University of Manchester (UK).
- Several **projects for Parallel Computing Resources** approved at the supercomputing facilities of CINECA, Italy, mainly in collaboration with Vincenzo Fiorentini, focusing on high-Tc superconductors, multiferroics, and diluted magnetic semiconductors.

Collaborations

- At the **University of Cagliari** the collaboration with the theoretical group of **Vincenzo Fiorentini** is extended to the study of *oxide cuprates and Mott insulators, doping-induced metal-insulating transition, the rare-earth oxides with high dielectric constant (LaAlO₃, LuO), the study of oxygen vacancies and defects in wide-gap insulators (e.g. HfO₂, ZnTe)*. Other collaborations are with the experimental group of **Samuele Sanna**, which is expert in growth and characterization of high-Tc oxide superconductors, within the context of a PRIN project studying the *coexistence of antiferromagnetism and superconductivity in cuprates*, and with **F. Bernardini** on the study of *Mn-doping in Si and GaAs*.
- I am an external collaborator of a project led by **Stefano Sanvito**, of the **Trinity College Dublin**, and funded by the Ireland Science Foundation, devoted to the *study and development, by first-principles calculations, of spintronic technology, aimed at integrating in a controllable manner both the spin and the charge of the electrons within a single device unit*.
- A long-term collaboration is with the group of **Prof. Nicola Spalding**, of the **University of California at Santa Barbara**, with whom *we elaborated the pseudo-SIC theory and applied it to a vast range of compounds*.
- An **international collaboration has been activated with a network of experimental groups from several European countries**, coordinated by groups of Physics Department (led by Prof. S. Siri) and CNR Materials Engineering (led by Prof. P. Nanni) at the University of Genova, Italy. This was established to attempt a collective effort in *developing multiferroic-based technology, including investigation of fundamental properties of known multiferroics, design, engineering and fabrication of novel devices made of single and double-phase ceramics, thin-films and layered heterostructures with enhanced multiferroic properties*.