VINCENZO FIORENTINI – FULL CV

(partial update : Sept 2021)

A – GENERAL

Born: Padova, Italy, on 5 Aprile 1960.

Citizenship and nationality: Italian.

Civil status: married. Two daughters (Isabella, 25; Beatrice, 23), one son (Giovanni, 14).

Current positions:

Scientific Counselor, Italian Embassy to Germany (07/2020-06/2024)
(on leave) Associate Professor, Italian scientific sector FIS-03–Physics of Matter, at the Facoltà di Scienze of Università degli Studi di Cagliari.
National habilitation to full professor, theoretical condensed matter physics (valid through 2028).

Home address

Via M. Besso 13, I-00191 ROMA, Italy
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Scientific coordinates:

Google Scholar: https://scholar.google.it/citations?user=_64ylnUAAAAJ
Scopus: https://www.scopus.com/authid/detail.uri?authorId=7004877164
ResearcherID: https://publons.com/researcher/E-4322-2010/
ResearchGate: https://www.researchgate.net/profile/Vincenzo_Fiorentini
ORCID: https://orcid.org/0000-0003-3794-8092

B – BRIEF SCIENTIFIC AND MANAGEMENT PROFILE

VF's activity is centered on the realistic theoretical description of the structural, electronic, vibrational, magnetic, dielectric, and polarization properties of solid-state systems. Typical topics have been: defects and impurities in semiconductors and oxides; dielectric and vibrational properties; low-dimensional nanostructures and interfaces; polarization and piezoelectricity applied to devices; fundamental processes (stress, reconstruction, adsorption and growth) at surfaces; correlation, magnetism, ferroelectricity, phase transitions, interface charge accumulation in oxides; thermal and electronic transport and thermoelectricity; high-throughput search and database extension for energy materials. Methodological developments included the density-functional stress

density, a method to compute dielectric tensors with polarization theory, self-energy corrections to density-functional theory, and recently variational self-interaction-free density functional methods. The main techniques used by VF are first-principles methods based on density-functional theory, and recently on post-DFT treatments for correlated systems. His activity is characterized by the prediction of observable quantities and effects, by continued comparison with experiment, and suggestions on the planning of specific experiments.

The main results of VF's research have been reported to date in around 130 publications on major refereed journals and about 10 invited and 20 contributed papers (mostly refereed) in proceedings or books. His scientific papers have around 10800 (ISI), 11500 (Scopus) and 15300 (Google Scholar, GS) citations. The Hirsch indexes [J. Hirsch, PNAS **102** 16569 (2005), Scientometrics **85**, 741 (2010)] (1989-today) are h=44 (ISI), 45 (Scopus), and 48 (GS). VF has held to date about 55 invited talks or lectures at international conferences and schools. VF is also included in the list of Top italian scientists of V.I.A. Academy, Manchester. A full publication list is attached, and is also available at `http://www.dsf.unica.it/~fiore/pub.pdf`. VF edited several books and journal special issues as proceedings of a major workshop series he has co-organized for 12 years, and is currently preparing three textbooks in computational physics, solid state physics, and elementary electromagnetism.

VF has been active in a number of consulting and hiring committees of several organizations and, to a lesser extent, in conference program and steering committees. A highlight of his activity in conference organizing is a very successful series of workshops in Sardinia between 1994 and 2006, where the very term "Computational Materials Science" was coined. Between Jan. 2004 and Jan. 2009 he headed the Sardinian Laboratory for Computational materials Science (whereof he was the proponent P.I.) of CNR/INFM, a 20-researcher organization among the top performers in computational materials physics in Italy, today an Operative Unit of CNR within the IOM institute. He has steadily managed his own research group (of size 3-5 people on average) and research grants/funding, tutoring and directing the work of about 30-40 students and post-docs, and receiving research funding from various national and international institutions for a gross total of roughly 3 MEuro. Besides early stays (3 years overall) in Freiburg and Berlin, he spent research periods abroad (1.5 years overall) as a Alexander-von-Humboldt fellow at the Walter Schottky Institute of the TU Munich, and as a Philips MC fellow at IMEC Leuven.

C – STUDIUM

7/1979 Maturità classica (high school license) at Liceo Classico "J. Stellini", Udine, Italy (final mark: 48/60).

7/1987 Laurea in Physics at Università degli Studi di Trieste, final mark 100/110. Thesis advisor: prof. A. Baldereschi.

10/1991 Completion of PhD thesis at Dipartimento di Fisica Teorica, Università degli Studi di Trieste. Tutor: prof. A. Baldereschi.

10/1992 Final PhD exam at Ministry of Research, Rome. Final mark: 'excellent'

D – EMPLOYMENT

D.1 – in Italy

2/1982-2/1983 Civil service at Vigili del Fuoco (Fire Guard), Udine

1/1989-10/1991 PhD student at Dipartimento di Fisica Teorica, Università degli Studi di Trieste, at the International center for Theoretical Physics.

12/1991-3/1992 Guest scientist, Dipartimento di Scienze Fisiche, Università degli Studi di Cagliari.

2/1993-4/2001 Ricercatore (lecturer, assistant professor) in the sector Condensed matter physics at Facoltà di Scienze, Università degli Studi di Cagliari.

from 4/2001 Associate University Professor, sector Physics of Matter, at Facoltà di Scienze MFN, Università degli Studi di Cagliari.

D.2 – abroad

11/1987-12/1988 Consultant scientist at Fraunhofer-Institut für Angewandte Festkörperphysik, Abt. Materialforschung, Freiburg i.B. (Germany), funded by a Fraunhofer Stipendium.

7/1990 Guest scientist at Fraunhofer-Institut für Angewandte Festkörperphysik, Abt. Materialforschung, Freiburg i.B. (Germany).

4/1992-10/1993 Temporary staff member of Fritz-Haber-Institut der Max-Planck-Gesellschaft, Abt. Theorie, Berlin (Germany), funded by a Max-Planck Stipendium.

Jul-Ott 1998, Jun-Jul 1999, Oct-Dec 2000 Alexander-von-Humboldt guest scholar at Walter Schottky Institut, Technische Universität München, Abt. Theoretische Halbleiterphysik, Garching (Germany), funded by an Alexander von Humboldt–Stiftung scholarship.

Dec 2005-Feb 2006, Nov 2006-Jan 2007 Marie Curie invited professor at Philips Research Leuven

E – TEACHING

As university lecturer and professor at Università di Cagliari:

1993-2000 Lectures on Condensed matter physics for Physicists.

1993-94 Lectures on Analytical Mechanics for Physicists.

1995-2002, and 2004-to date Full course on Computational methods of physics, for Physicists.

2015-to date Full course on "Fisica 2" – Basic electromagnetism for Electronic Engineers.

2015-to date Full online e-course on "Fisica 2" – Basic electromagnetism for Electronic Engineers.

1996-97 Full course on Mathematics, Diploma in Economics.

1997-2003 Full course on Solid state physics, Diploma in Materials Science.

1998-2003 Full course on Surface Physics, for Physicists.

2001-2002, 2009-to date Full course on Foundations of computational physics, for Physicists.

1998-99 Lectures of Semiconductor Physics, for Physicists.

2002-2003 Full course of Semiconductor Physics, for Physicists.

2002-2010 Full course on Computational physics, for Physicists.

2003-2008 Full course on Computational condensed matter physics, for Physicists.

2004-2010 Full course on Solid state physics, for Physicists.

2010-2014 Full course on Condensed matter physics for Physicists.

Since 1993 Advisor of about 30 laurea (Master/Diplom-like) theses, 4 Bachelor, and about 12 PhD theses.

1995 Invited lectures on "Pseudopotentials in electronic structure applications", Workshop on Computational Methods in Material Science and Engineering, ICTP Trieste.

2000 Invited lectures on "Spontaneous and piezoelectric polarization in semiconductors: conceptual aspects and applications", International School of Semiconductor Physics, Jaszowiecz (Polonia).

2010 Invited lecture on "Ab initio description of correlation-induced transitions in solids", CNR-UCSB Workshop "Aquila Initiative for Ferroics", L'Aquila (Italy).

2011 Invited lectures on "Topics in the ab initio theory of oxides", "Workshop on Advanced Oxide Interfaces" at International Center for Theoretical Physics, Trieste.

F – RESEARCH MANAGEMENT AND ORGANIZATION

F.1 – Management of projects and personnel

2004-2009 Director of SLACS, Sardinian LAboratory for Computational Materials Science.

1993 to date Scientific advisor of post-doc researchers for approximately 60 man-years within approximately 15 different projects.

2017-onward PI in Project *Multiphysics approach to thermoelectricity*, Fonsazione Sardegna-Uni Cagliari.

2012-2016 Local scientific responsible in the national research project funded by Ministry of research (MIUR-PRIN 2010) "Oxide".

2002-2007 PI of a MIUR "Ritorno dei Cervelli" contract at Università di Cagliari.

2006-2009 Recipient of a Fondazione Banco di Sardegna grant on "Correlated multiferroics".

2008-2010 Recipient of a Fondazione Banco di Sardegna grant on "Spintronic devices based on manganites".

2009-2013 Local scientific responsible at CNR IOM-SLACS Cagliari for the Research Project "NEWDFESCM: New density functionals for the electronic structure of complex materials.", funded by the Italian Institute of Technology.

2008-2012 Local scientific responsible at CNR SLACS for the EU-NPM Research Project "ATHENA: Advanced theories for functional oxides: new routes to handle the devices of the future", funded by the EU 7 FP.

2008-2012 Local scientific responsible at CNR SLACS for the EU-SMP Research Project "OxIDe: Oxide interface design", funded by the EU 7 FP.

1993-96 Local scientific responsible at Università di Cagliari for the Focused Fundamental Research Project "LASBE" on III-V nitrides and their nanostructures, funded by the EU Brite-EURAM II program.

1997-1999 PI of the advanced project (PAIS) "Theory of metallic contacts on nitrides and oxides" funded by the Semiconductors division of National Institute for the Physics of Matter (INFM).

1999-2001 Local scientific responsible in the national research project funded by Ministry of research (MIUR-Cofin 1999) "Fisica e tecnologia di eterostrutture a nitruri".

2000-2002 Local scientific responsible in the national research project funded by Ministry of research (MIUR-Cofin 2000) "Diffusione di non-equilibrio in nanostrutture a base silicio".

2001-2003 Local scientific responsible in the national research project funded by Ministry of research (MIUR-Cofin 2001) "Caratterizzazione ottica e strutturale e trattamenti post-crescita di eterostrutture InGaAsN / GaAs".

2002-2004 Local scientific responsible in the national research project funded by Ministry of research (MIUR-Cofin 2002) "Diffusione e clustering di droganti in silicio cristallino".

2005-2007 National PI in the national research project funded by Ministry of research (MIUR-Cofin 2005) "Coexistence of magnetism and metallicity in oxide superconductors".

2007-2009 Co-responsible for "Obiettivo Realizzativo 7.1, *Ab initio study of innovative materials for spintronics and electronics at the nanoscale*, of project "Cybersar" funded by MIUR at Uni CA under the PON program.

2001-2004 Responsible for theoretical activity within INFM-MDM Lab in the project INVEST on the epitaxy of high-κ oxides on Si, funded by the EU.

2001-2005 PI and scientific responsible for the project Fondo Integrativo Ricerca di Base (FIRB) "Basi microscopiche della morfologia di film metallici epitassiali".

2003-2004 Local scientific responsible of the advanced project (PAIS) "Rare-earth high-k oxides for Si microelectronics" funded by the Semiconductors division of National Institute for the Physics of Matter (INFM).

1999 to date PI in many supercomputing projects (on average 2-3 yearly, at CINECA or CASPUR)

F.2 – Conference organization

1994-2005 Co-organizer of the Computational Materials Science Workshop, Cagliari.

1995-98 Member of Program committee of the series European Gallium Nitride Workshops.

1997-2000 Member of Program committee of International Conference on Nitride Semiconductors.

1999 Program chair of symposium "Nitride semiconductors" at INFM-Meeting (Catania, Italy)

1999-2003 Member of Program and Advisory Committee of International Symposium on Blue Light Emitting Devices.

1999 Member of Program and Advisory Committee of International Conference on Ternary and Multinary Compounds.

F.3 – Scientific evaluation committees

passim Member of selection committees for grants, post-doc positions, admission to PhD school, final PhD examinations, etc.

1998 Member of the committee for the hiring of the head of a junior independent group at Fritz-Haber-Institut, Berlin.

1996-97 Project referee for the Schwerpunktprogramm *Gruppe III-Nitride und ihre Heterostrukturen* of the Deutsche Forschungsgemeinschaft.

1997-2002 Member of the committee for local funding of physics research at Università degli Studi di Cagliari.

2002 Consultant referee for the Swiss National Science Foundation.

2005-2008 Consultant to the Ministry of Industry.

2005 Consultant referee for the Steering Committee on Research of the Ministry of University and Research.

2007 Member of the committee for the hiring of an assistant professor at University of Padova.

2008-onward Consultant referee for the Estonian National Science Foundation.

2011-onward Consultant referee for the Romanian National Science Foundation.

2010 Consultant to Veneto Innovazione (regional funding agency).

2011-12 Consultant to Ministry of University and research (industrial project evaluation)

2012 Consultant to Ministry of University and research (VQR, FIRB, SIR, FIR, EUROSTAR evaluation)

2012 Consultant to CNR (FIRB project evaluation)

2013 Consultant to Science Foundation Ireland (PI-award review)

F.4 – Other management and service activities

1992 to date Referee for Nature, Physical Review Letters, Physical Review B, Applied Physics Letters, Europhysics Letters, Surface Science, Journal of Applied Physics, physics status solidi, Computational Materials Science, European Physical Journal B, and occasional others.

1995-2007 Coordinator of ERASMUS/SOCRATES activities for physics at Università di Cagliari.

2000-2003 Elected member of the Executive Committee of the Semiconductors division of INFM.

2001-2006 Editorial Board member of International Journal of Theoretical and Computational Chemistry.

2013-2014 Member of international scientific committee of 7th WSEAS International Conference on Materials Science (MATERIALS '14), Cambridge, MA, USA

G – INVITED TALKS AT INTERNATIONAL CONFERENCES

G.1 – Complete list

Besides several tens of contributed talks or posters at national and international congresses and several invited seminars at various institutions, I held well over 50 invited talks to date at international conferences or schools. Many further invited talks have been held by coauthors of the relevant works. The invited talks I have given in person are:

1991 II Italian-Swiss Workshop on Computational Condensed Matter Physics, S. Margherita di Pula (CA) (invited talk).

1992 III Italian-Swiss Workshop on Computational Condensed Matter Physics, S. Margherita di Pula (CA) (invited talk).

1993 Convegno GNSM "Fisica Teorica e Struttura della Materia", Fai della Paganella (TN) (invited talk).

1994 Miniworkshop on Total Energy and Force Methods, Copenhagen (invited participant and speaker).

1994 Frühjahrstagung der Deutsche Physikalische Gesellschaft, Münster (invited talk).

1994 Workshop on Computational Material Science, Brindisi (invited talk).

1995 Workshop on Computational Methods in Material Science and Engineering, ICTP Trieste (invited lectures).

1995 Workshop on Computer Simulation of Crystal and Overlayer Growth, Lyon (invited participant and speaker).

1996 MRS Fall Meeting, Boston (invited talk)

1997 Congresso Nazionale INFM, Chia (CA) (invited talk).

1997 Workshop on First-principles Theory of Ferroelectricity, CECAM Lyon (invited participant and speaker).

1997 Workshop on Simulation of Silica Glasses, CECAM Lyon (invited participant and speaker).

1998 Max-Planck Symposium on Surface Morphology, Interfaces, and Growth of III-V Nitrides, Ringberg, Germany (invited talk).

1998 Congresso Nazionale INFM, Rimini (invited talk).

1999 Workshop on Computational Materials Science at the Abdus Salam International Centre for Theoretical Physics, Trieste, Italy (invited talk).

1999 Convegno GNSM "Fisica Teorica e Struttura della Materia", Fai della Paganella (TN) (invited talk).

1999 International Conference on the Formation of Semiconductor Interfaces, Göteborg, Sweden (invited talk).

1999 Solid State Devices and Materials Conference, Tokio, Japan (invited talk).

2000 International Conference on Ternary and Multinary Semiconductors, Hsin-Chu, Taiwan (invited talk).

2000 International School of Semiconductor Physics, Jasowiecz, Poland (invited lecture).

2000 Workshop on Growth, morphology and magnetic properties of epitaxial metallic systems, CECAM Lyon (invited participant and speaker).

2000 PSI-K2000 - Ab initio (from Electronic Structure) Calculations of Complex Processes in Materials, Schwäbisch Gmünd, Germany (invited talk).

2001 MURI-ONR Polaris project review, Cornell University, USA (invited talk).

2001 E-MRS - European Materials Research Society Meeting, Strasbourg, Francia (invited talk).

2001 Max-Planck Symposium and Heraeus Seminar on Electronic origin of magnetoelastic anisotropy and stress in atomic layers, Ringberg, Germany (invited talk).

2002 International Symposium on Blue-Light-Emitting Devices (ISBLED-2), Cordoba, Spagna (invited talk).

2002 International Conference on Extended Defects in Semiconductors, Bologna, Italy (invited talk).

2002 Italian Physical Society General Congress, Alghero, Italy (invited talk).

2002 ChIPPS 2002 - Challenges in Predictive Process Simulation, Prague, Chzekia (invited talk).

2003 ESF Workshop on Submicron gate oxides in Si technology, Zürich, Svizzera (invited talk).

2004 CECAM workshop on Atomic processes at Si/oxide interfaces, Lyon, Francia (invited participant and speaker).

2005 ESF Workshop on Rare-earth oxides, S. Remo, Italy (invited participant and speaker).

2005 NATO Workshop on Defects in High-k oxides, S. Petersburg, Russia (invited talk).

2005 Italian Physical Society General Congress, Catania, Italy (invited talk).

2006 E-MRS Spring Meeting, Nice (invited talk).

2006 ElectroChemical Society of America, Gate Stacks Symposium, Cancun, Mexico (invited talk).

2006 Workshop "Modeling at the nanoscale", Palau, Italy (invited talk).

2008 e-science conference 2008, Naples, Italy (invited talk).

2010 AQUIFER - Aquila initiative on ferroics, L'Aquila, Italy (invited lecturer; resident tutoring scientist).

2010 Workshop "Emergent trends in advanced correlated materials", Capri, Italy (invited talk).

2011 Thomas Young Center Soirée "Correlated materials with DFT ?", London, UK (invited speaker)

2011 Workshop on Advanced Oxide Interfaces, International Center for Theoretical Physics, Trieste, Italy (invited lecturer)

2011 Workshop "Frontiers in fundamental physics", Università di Udine, Udine, Italy (invited speaker)

2014 E-MRS Fall Meeting, Symposium Functional perovskite systems, Warsaw, Poland (invited speaker)

2016 Deutsche Physikalische Gesellschaft, Spring Meeting of Condensed Matter Division, Regensburg, Germany (invited speaker)

2016 Energy materials nanotechnology meeting, Dubrovnik, Croatia (invited speaker)

2016 CIMTEC symposium on multiferroics, Perugia, Italy (invited speaker)

2017 Energy materials nanotechnology meeting "Density functional theory and its applications", Dubai, (invited speaker)

2018 CIMTEC Symposium on functional oxides, Perugia, Italy (invited speaker)

2018 E-MRS Fall Meeting, Symp.I, Warsaw, Poland (invited speaker)

2018 E-MRS Fall Meeting, Symp.J, Warsaw, Poland (invited speaker)

2018 PyCon Sardegna (invited speaker)

2018 MRS Fall Meeting, Symp EP08, Boston (invited speaker)

2019 Nanoinnovation 2019, Rome, Italy, Symp "Towards Exascale Supercomputers for Nanotechnology" (invited speaker)

G.2 – A selection of invited talks

MRS Fall Meeting 1996
Max-Planck Symposium 1998
"Total-Energy" Workshop 1999
Psi-k Conference 2000
CHIPPS 2002
ESF workshop on rare-earth oxides 2005
SIF 2005
AQUIFER 2010
ETACM 2010
DPG 2016
E-MRS 2018

H – AWARDS AND GRANTS

2013 "Abilitazione" to full professor, theoretical condensed matter physics

2017 Research prize of University of Cagliari

2013 Research prize of University of Cagliari

2012 Research prize of Regione Sardegna

2011 Research prize of University of Cagliari

2005-2006 Marie Curie invited professor at Philips Research Leuven

1998-2000 Alexander von Humboldt Research Fellowship

2017 Fondazione Sardegna grant

2006 Fondazione Banco di Sardegna grant in research

2008 Fondazione Banco di Sardegna grant in research

2010 Fondazione Banco di Sardegna grant in research

2009 EU NMP Research Grant on perovskite oxides

2008 EU NMP Research Grant on correlation in oxides

2005 EU FP6 Coordination action "CADRES" on defects in Si (expert-group coordinator).

2008 IIT Research Grant on new density functionals

1994-96 EEC Brite-EURAM Research Grant on III-V Nitrides

1999-2000 MURST-Cofin grant on nitride nanostructures

2000-2001 MURST-Cofin grant on impurities in Si

2001-2003 MIUR-PRIN grant on GaAsN alloys

2002-2004 MIUR-PRIN grant on impurities in Si

2005-2007 MIUR-PRIN grant on oxide superconductors

2012-2016 MIUR-PRIN grant on oxide interfaces

1997-99 PAIS-INFM grant on metal-nitride contacts

2003-2004 PAIS-INFM grant on rare-earth oxides

2002-2005 MIUR-FIRB grant on the epitaxial growth of metals

2001-2004 EU grant on high-κ oxides on Si

1997-99 Regione Sardegna grant on III-V nitrides

1999-2001 Regione Sardegna grant on parallel computing

1999-2003 Università di Cagliari personnel grant on III-V nitrides

2003-2007 Scientific responsible of MIUR-"Cervelli per la ricerca" grant

1993 to date Supercomputing grants

I – MEMBERSHIP IN SCIENTIFIC SOCIETIES

1989-2003 Deutsche Physikalische Gesellschaft.

2005-onward CNR ("associato")

2005-2009 American Physical Society

2012-2017 Società Italiana di Fisica

Vincenzo Fiorentini

Publication List

(updated : Oct 2021)

A – Books [3], edited books [2] and Special Issues [3]

1. **V. Fiorentini** and P. Alippi
   Fondamenti di fisica dei solidi
   (in preparation, 2019)

2. **V. Fiorentini** and F. Ricci
   Fondamenti di fisica computazionale
   (in preparation, 2019)

3. **V. Fiorentini** and M. B. Maccioni
   Appunti di fisica generale: elettromagnetismo
   (in preparation, 2019)

4. **V. Fiorentini** and F. Meloni (eds.), *Advances in Computational Materials Science* (Società Italiana di Fisica, Bologna 1997), 119 pages.

5. **V. Fiorentini** and F. Meloni (eds.), *Advances in Computational Materials Science – II* (Società Italiana di Fisica, Bologna 1998), 122 pages.

6. **V. Fiorentini**, F. Meloni, and P. Ruggerone, guest editors: *Computational Materials Science IX*, Comput. Mat. Sci. **20**, Nos. 3-4 (2001).

7. P. Ruggerone, **V. Fiorentini**, and F. Meloni, guest editors: *Computational Materials Science X*, Comput. Mat. Sci. **22**, Nos. 3-4 (2002).

8. P. Ruggerone, **V. Fiorentini**, and F. Meloni, guest editors: *Computational Materials Science*, Comput. Mat. Sci. **30**, Nos. 1-2 (2004).

B – Papers on peer-reviewed international journals [132]

1. **V. Fiorentini** and A. Baldereschi:
   Interpretation of double acceptor spectra in Ge,
   Solid State Commun. **69**, 953-958 (1989).

2. **V. Fiorentini**:
   Self-consistent DFT calculations of electronic states in superlattices and quantum wells with arbitrary compositional and doping profiles,
   Semicond. Sci. Technol. **5**, 211-217 (1990).

3. **V. Fiorentini**:
   Semiconductor band structures at zero pressure,
   Phys. Rev. B **46**, 2086-2091 (1992).

4. **V. Fiorentini** and A. Baldereschi:
   Semiempirical self-energy correction to LDA bands of semiconductors, and a scaling law for the scissor operator,
   J. Phys. Condensed Matter **4**, 5967-5976 (1992).

5. **V. Fiorentini**:
   A note on ab-initio semiconductor band structures,
   Solid State Commun. **81**, 871-875 (1992).

6. **V. Fiorentini**, M. Methfessel and M. Scheffler:
   Electronic and structural properties of GaN by the full-potential LMTO method: the role of the d electrons,
   Phys. Rev. B **47**, 13353-13362 (1993).

7. **V. Fiorentini**, M. Methfessel and M. Scheffler:
   Reconstruction mechanism of fcc transition-metal (001) surfaces,
   Phys. Rev. Lett. **71**, 1051-1054 (1993).

8. S. Oppo, **V. Fiorentini** and M. Scheffler:
   Theory of adsorption and surfactant effect of Sb on Ag (111),
   Phys. Rev. Lett. **71**, 2437-2440 (1993).

9. **V. Fiorentini**, S. Oppo, and M. Scheffler:
   Towards an understanding of surfactant action on the epitaxial growth of metals: the case of Sb on Ag (111),
   Appl. Phys. A **60**, 399-402 (1995).

10. **V. Fiorentini**:
    Effective-mass single and double acceptor spectra in GaAs,
    Phys. Rev. B **51**, 10161-10163 (1995)

11. **V. Fiorentini** and A. Baldereschi:
    Dielectric scaling of the self-energy scissor operator in semiconductors and insulators,
    Phys. Rev. B **51**, 17196-17198 (1995)

12. A. Bosin, **V. Fiorentini**, A. Lastri and G. B. Bachelet:
    Local norm-conserving pseudohamiltonians,
    Phys. Rev. A **52**, 236-257 (1995)

13. **V. Fiorentini** and M. Methfessel:
    Extracting convergent surface energies from slab calculations,
    J. Phys. Cond. Matter **8**, 6525-6529 (1996).

14. **V. Fiorentini**, D. Fois and S. Oppo:
    Inhibited Al diffusion and growth roughening of Ga-coated Al (100),
    Phys. Rev. Lett. **77**, 695-698 (1996).

15. A. Filippetti and **V. Fiorentini**:
    Reconstructions of Ir (100) and (110): an ab initio study,
    Surface Science **377**, 112-116 (1997).

16. F. Bernardini, **V. Fiorentini**, and A. Bosin:
    Theoretical evidence for efficient p-type doping of GaN using beryllium,
    Appl. Phys. Lett. **70**, 2990-2992 (1997).

17. C. M. Carbonaro, **V. Fiorentini**, and S. Massidda:
Ab initio study of oxygen vacancies in α-quartz,
J. Non-Cryst. Solids **221**, 89-96 (1997).

18. F. Bernardini, **V. Fiorentini**, and D. Vanderbilt:
Spontaneous polarization and piezoelectric constants of III-V nitrides,
Phys. Rev. B **56**, R10024-R10027 (1997).

19. F. Bernardini, **V. Fiorentini**, and D. Vanderbilt:
Polarization-based calculation of the dielectric tensor of polar crystals,
Phys. Rev. Lett. **79**, 3958-3961 (1997).

20. F. Bernardini and **V. Fiorentini**:
Macroscopic polarization and band offsets at nitride heterojunctions,
Phys. Rev. B **57**, R9427-R9430 (1998).

21. S. Oppo and **V. Fiorentini**:
No in-plane reconstruction of Cu (001),
Phys. Rev. Lett. **81**, 4278-4278 (1998).

22. F. Bernardini and **V. Fiorentini**:
Electronic dielectric constants of insulators by the polarization method,
Phys. Rev. B **58**, 15292-15295 (1998).

23. A. Filippetti, **V. Fiorentini**, G. Cappellini, and A. Bosin:
Ionicity and relaxation behavior at III-V nitride surfaces,
phys. stat. sol. (a) **170**, 265-268 (1998).

24. A. Fara, F. Bernardini, and **V. Fiorentini**:
Theoretical evidence for the semi-insulating character of AlN,
J. Appl. Phys. **85**, 2001-2003 (1999).

25. U. Hansen, P. Vogl, and **V. Fiorentini**:
Atomistic modelling of large-scale metal film growth fronts,
Phys. Rev. B **59**, R7856-R7859 (1999).

26. 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**, 8026-8031 (1999).

27. F. Della Sala, A. Di Carlo, P. Lugli, F. Bernardini, **V. Fiorentini**, R. Scholz, and J.-M. Jancu:
Free-carrier screening of polarization fields in wurtzite GaN/InGaN laser structures,
Appl. Phys. Lett. **74**, 2002-2004 (1999).

28. U. Hansen, P. Vogl, and **V. Fiorentini**:
Quasi-harmonic vs. "exact" surface free energies of Al: a systematic study employing a new interatomic potential,
Phys. Rev. B **60**, 5055-5064 (1999).

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