CURRICULUM VITAE

Gian-Marco RIGNANESE

Address:	Institute of Condensed Matter and Nanosciences (IMCN)		
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	Belgium	E-mail:	gian-marco.rignanese@uclouvain.be
Nationality:	Belgian	Date of birth:	7 February 1972
Marital Status:	Married, two daughters	Place of birth:	Charleroi (Belgium)
Languages:	Fluent in French, English, Italian; some knowledge in Dutch and Chinese		

Overview

Academic degrees

– Ph. D. in Applied Sciences, (UCL, June 1998).
– B. Sc. in Engineering - Applied Physics ("Ingénieur Civil Physicien", UCL, July 1994)

Current position

– Senior Research Associate of the Fund for Scientific Research (F.R.S.-FNRS Belgium)
– Part-time Professor ("Professeur à temps partiel", UCL)

Research activities

– Computer simulation of different properties of materials using *ab initio* techniques (Density Functional Theory, *GW* approximation, Bethe-Salpeter Equation) in the framework of the ABINIT package (http://www.abinit.org).
– Study of structural, electronic, dynamical, and dielectric properties of transition metal oxides and silicates (high-κ materials) and their interface with silicon.
– Study of optical properties of transparent conducting oxides.
– High-Performance Computing.

Scientific output

– 66 publications (52 journal articles, 5 book chapters, 8 conference papers, 1 popularization article)
Scopus (h=24, >4200 citations) / Web of Science (h=24, >4000 citations) / Google Scholar (h=26, >5100 citations)
– 123 contributions to professional meetings (73 oral communications [34 invited talks], 50 posters)
– 34 seminars and 19 invited lectures

Academic activities

– Teaching: lectures at the UCL (presently, FSAB1503, MAPR1492, MAPR2014)
– Supervision of 9 PhD students since 2004 and 6 Master students since 2009

Administrative activities and services

– Head of the Nanoscopic Physics (NAPS) division of the Institute of Condensed Matter and Nanosciences (IMCN)
– Member of the Conseil de Direction of Institut de Calcul Intensif et Stockage de Masse (CISM) since 2006.
– Representative of the Ecole Polytechnique de Louvain (EPL) to the `Comité de la Bibliothèque des Sciences et Technologies' since 2012.
– Representative of the IMCN to the `Comité Sectoriel du Système d'Information pour les Sciences Exactes' since 2012.
– Member of 11 PhD examination board since 2002.
– Organizer or member of the program committee of 15 meetings since 2002.
– Editor of the Journal of Computational Methods in Physics (Open Access) since 2013.
– Referee for 7 international peer-reviewed journals including Phys. Rev. Lett., Appl. Phys. Lett, Phys. Rev. B, Langmuir.

Awards and Grants

– Firmin Van Brée Fellow 1998-99 of the Hoover Foundation of the Belgian American Educational Foundation
– Grantee of the Fulbright Program 1998-99 of the Commission for Educational exchange
– Holder of a 'Bourse post-doctorale de recherche scientifique 1998-99' of the 'Université Catholique de Louvain'
– Holder of a 'Bourse scientifique pour bref séjour à l'étranger 1998' of the FNRS-Belgium
– Award winner of the 'Concours des Bourses de Voyages 1996' of the 'Communauté Française de Belgique'

1. Career sketch

Education

– **September 1990-July 1994**: Engineering Student, UCL.
  June 1990, grande distinction (81%).
  June 1991, grande distinction (83%).
  June 1992, la plus grande distinction (86%).
  July 1993, la plus grande distinction (88%).
  July 1994, la plus grande distinction (88%).
– **October 1994-September 1998**: Ph.D. Student at the UCL in the PCPM ab initio Group (supervisor: Prof. X. Gonze).
  Doctoral dissertation:"Firs-Principles Molecular Dynamics Study of SiO_2: Surface and Interface with Si"

Research

– **October 1994-September 1998**: Research Fellow ("Aspirant") of the FNRS-Belgium
– **August 1996-December 1996**: Software Development Consultant for the PATP (Parallel Application Technology Project), collaboration between CRAY RESEARCH and Ecole Polytechnique Fédérale de Lausanne(EPFL), for the Institut Romand de Recherche Numérique en Physique des Matériaux (IRRMA).
– **October 1998-September 1999**: Postdoctoral Fellow in the Theoretical Condensed Matter Physics Group of Prof. S. G. Louie, Departement of Physics, University of California at Berkeley, Berkeley, USA.
– **October 1998-September 1999**: Visiting Scholar in the Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, USA.
– **October 1999-September 2003**: Postdoctoral Fellow in the PCPM ab initio Group as
  Postdoctoral Researcher of the UCL (October 1999-September 2000)
  Scientific Research Worker ("Collaborateur scientifique") of the FNRS-Belgium (October 2000-September 2001)
  Postdoctoral Researcher ("Chargé de recherche") of the FNRS-Belgium (October 2001-September 2003)
– **October 2003-present**: Permanent Staff in the Louvain-la-Neuve ab initio Group as
  Research Associate ("Chercheur qualifié") of the FNRS-Belgium (October 2003-September 2011)
  Senior Research Associate ("Maître de recherches") of the FNRS-Belgium (October 2011-present)

Teaching

– **September 2002-September 2003**: Invited Lecturer ("Chargé de cours invité"), Université de Liège (ULg).
– **September 2003-September 2011**: Part-time Assistant Professor ("Chargé de cours à temps partiel"), UCL.
– **September 2011-Present**: Part-time Professor ("Professeur à temps partiel"), UCL.

2. Teaching Experience

As teaching assitant

– 1992-1993: Algebra for first-year engineering students at the UCL.
– 1992-1993: Thermodynamics for second-year engineering students at the UCL.
– 1993-1995: Physical-Chemistry for first-year engineering students at the UCL.
– 1996-1997: `Propriétés des Matériaux' (MAPR2492) for third- and fourth-year engineering students at the UCL.
– 1996-2001: Integrated Exercises for second-year engineering students at the UCL.
– 2001-2002: Physics (FSA1630C) for engineering students at the UCL.
– 2003-2005: `Introduction à la Physique des Matériaux' (MAPR2110) for third-year engineering students at the UCL.

As teacher

– 2002-2003: Quantum Chemistry (CHIM208) for second-year chemistry students at the ULg (30 hours).
– 2005-2006: `Introduction à la Physique des Matériaux' (LMAPR2110) for third-year engineering students at the UCL (shared with J.-C. Charlier and X. Gonze, personnal charge 15 hours)
– 2006-2013 : `Matière Condensée' (LPHY1342) for third-year physics students at the UCL (shared with L. Piraux, personal charge 15 hours)
– 2006-present. : 'Physique des Matériaux' (LMAPR1492) for third-year engineering students at the UCL (shared with L. Piraux, personal charge 12.5 hours)
– 2007-present : `Physique des Matériaux Fonctionnels' (LMAPR2014) for fourth-year engineering students at the UCL (shared with X. Gonze and L. Piraux, personal charge 12.5 hours)
– 2010-present : `Projet 3' (LFSAB1503) for second-year engineering students at the UCL (shared with J.-C. Charlier, X. Gonze, and J.-P. Raskin, personal charge 15 hours)
– 2013-present : `Simulations atomistiques et nanoscopiques' (LMAPR2451) for fourth-year engineering students at the UCL (shared with X. Gonze and J.-C. Charlier, personal charge 10 hours)

3. Supervision of students and participation to examination boards

– Supervisor of 9 PhD students since 2004
(1) M. Giantomassi, PhD (Sep 2005-May 2009)
(2) S. M.-M. Dubois, PhD (Oct 2004-Feb 2010)
(3) T. Rangel, PhD (Apr 2007-Aug 2011)
(4) K. Sankaran, PhD (Oct 2008-Sep 2012)
(5) D. Kecik, PhD @ EPFL (Nov 2010-January 2013)
(6) A. Miglio, PhD (Feb 2009-Jun 2013)
(7) O. Bitchaeva, PhD (Nov 2010-...)
(8) S. Poyyapakkam Ramkumar (Oct 2013-…)
(9) N. Dardenne (Mar 2014-…)

– Supervisor of 6 Master students since 2009
(1) A. Pairet, Master Ingénieur civil en chimie et science des matériaux (Sep 2009-Sep 2010)
(2) O. Poncelet, Master Ingénieur civil physicien (Sep 2010-Jun 2011)
(3) N. Butaije, Master Ingénieur civil physicien (Sep 2010-Sep 2011)
(4) T. Münstermann, Master Ingénieur civil physicien (Sep 2011-Jun 2012)
(5) G. Baudoin, Master Ingénieur civil physicien (Sep 2012-Sep 2013)
(6) N. Dardenne, Master complémentaire en nanotechnologie (Sep 2012-Sep 2013)

– Member of 11 PhD examination board since 2002
(1) F. Detraux (UCL, Nov 2002)
(2) M. Verstraete (UCL, Jul 2005),
(3) Y. Bertholet (UCL, Oct 2006)
(4) F. Devynck (EPFL, May 2008)
(5) P.-Y. Prodhomme (CEA-Grenoble, Jun 2008)
(6) E. Bousquet (ULg, Sep 2008)
(7) P. Darancet (UJF-Grenoble, Dec 2008)
(8) M. Scarrozza (KUL, Jan 2011)
(9) X. Declerck (UCL, Feb 2013)
(10) D. Waroquiers (UCL, Feb 2013)
(11) K. Noori (Oxford, Oct 2013)

– Member of 1 “Habilitation” examination board since 2014: F. Bruneval (Lyon, June 2014)

– Member of the “comité d’encadrement” of E. Bousquet (ULg, October 2004-September 2008), X. Declerck (UCL, October 2008-February 2013), D. Waroquier (UCL, October 2008-February 2013), N. Leconte (UCL, October 2009-...), S.O. Guillaume (FUNDP, October 2010-...), S. Poncé (UCL, October 2010-...), Y. Gillet (UCL, October 2012-...)

– Member of the examination board (“lecteur”) of N. Benyahia (UCL, Ingénieur Civil, Jun 1996), M. Iker (UCL, Ingénieur Civil, Jun 2004), S. M.-M. Dubois (UCL, Ingénieur Civil, Jun 2004), S. André (UCL, Ingénieur Civil, Jun 2007), X. Declerck (UCL, Ingénieur Civil, Jun 2008), E. Goossens (UCL, Ingénieur Civil, Jun 2008), D. Waroquiers (UCL, Ingénieur Civil, Jun 2008), N. Leconte (UCL, Ingénieur Civil, Jun 2009), R. Cai (UCL, Ingénieur Civil, Jun 2010), M. Haslinger (UCL, Ingénieur Civil, Jun 2011), E. van Caloen (UCL, Ingénieur Civil, Jun 2011), Y. Gillet (UCL, Ingénieur Civil, Jun 2012), T. Legat (UCL, Ingénieur Civil, Sep 2013), R. Haouari (UCL, Ingénieur Civil, Jun 2014), S. Toussaint (UCL, Ingénieur Civil, Jun 2014), B. Van Troeye (UCL, Ingénieur Civil, Jun 2014).

4. Services to the academic and scientific communities

– Head of the Nanoscopic Physics (NAPS) division of the IMCN since 2013

– Representative of the IMCN to the `Comité Sectoriel du Système d’Information pour les Sciences Exactes’ since 2012.

– Representative of the EPL to the `Comité Sectoriel du Système de la Bibliothèque des Sciences et Technologies (BST)’ since 2012.

– Member of the Conseil de Direction of Institut de Calcul Intensif et Stockage de Masse (CISM) since 2006.

– Referee for Physical Review Letters, Applied Physics Letters, Physical Review B, Langmuir, Surfarce Science, European Physics Journal B and Materials Research Bulletin.

– Representative of the MAPR Department with respect to the `Bibliothèque des Sciences et Technologies’ (2004-2011).

– Academic Secretary of MAPR Department (2006-2009).

– Representative of the MAPR Department for the ‘Commission Informatique Facultaire’ (2002-2003).

– Representative of the Scientific Staff for the ‘Bureau de Département MAPR’ (1995-1997).

– Representative of the Scientific Staff for the ‘Conseil de Département MAPR’ (1995-1997).

– Representative of the Scientific Staff for the ‘Conseil de Faculté’ (1995-1997).

– Representative of the Scientific Staff for the ‘Commission des Diplômes Départementale’ (1997-1998).

5. Organisation of scientific meetings

1. Member of the local organizing committee of the “First International ABINIT developer workshop”,
   Louvain-la-Neuve (Belgium), 6-8 November 2002.
   http://www.abinit.org/community/events
2. Organizer of the 2003 annual meeting of the “Exciting” European Research and Training Network
   Louvain-la-Neuve (Belgium), 14-16 April 2003.
   http://www.abinit.org/exciting
3. Organizer of the “Second International ABINIT developer workshop”,
   Paris (France), 10-12 May 2004.
   http://www.abinit.org/community/events
4. Organizer of the “11th Nanoquanta-ETSF Workshop on Electronic Excitations: A decade of applications of the BSE”,
   Houffalize (Belgium), 19-22 September 2006.
   http://www.etsf.eu/etsf_workshop_archive/06
5. Organizer of the CECAM Tutorial “Electronic excitations and spectroscopies: theory and codes”
   Lyon (France), 11-15 December 2006.
   http://www.cecam.org/workshop-123.html
6. Organizer of the “12th Nanoquanta-ETSF Workshop on Electronic Excitations: TDDFT Advances and Prospects”,
   Aussois (France), 18-22 September 2007.
   http://www.etsf.eu/etsf_workshop_archive/07
7. Organizer of the CECAM Tutorial “Theoretical Spectroscopy Lectures: theory and codes”
   Lyon (France), 10-14 December 2007.
   http://www.cecam.org/workshop-193.html
8. Organizer of the “13th Nanoquanta-ETSF Conference on Electronic Excitations: Theoretical Spectroscopy and Quantum Transport”,
   Pugnochiuso-Vieste (Italy), 23-27 September 2008.
   http://www.etsf.eu/etsf_workshop_archive/08
9. Organizer of the CECAM Tutorial “Theoretical Spectroscopy Lectures: theory and codes”
   Zurich (Switzerland), 25-29 May 2009.
   http://www.cecam.org/workshop-314.html
10. Organizer of the “14th Nanoquanta-ETSF Conference on Electronic Excitations: Ab-initio tools for the characterization of nanostructures”,
    Evora (Portugal), 14-19 September 2009.
    http://www.tddft.org/ETSF2009
11. Organizer of the “15th Nanoquanta-ETSF Conference on Electronic Excitations::New Frontiers in Theoretical Spectroscopy and Quantum Transport”,
    Berlin (Germany), 12-15 October 2010.
    http://etsf.polytechnique.fr/etsfconference2010/
12. Member of the local organizing committee of the “Fifth International ABINIT developer workshop”,
    Han-sur-Lesse (Belgium), 11-14 April 2011.
    http://www.abinit.org/community/events
13. Organizer of the CECAM Tutorial “Theoretical Spectroscopy Lectures: theory and codes”
    Lausanne (Switzerland), 2-6 May 2011.
    http://www.cecam.org/workshop-504.html
14. Organizer of the CECAM Tutorial “Theoretical Spectroscopy Lectures: theory and codes”
    Lausanne (Switzerland), 13-17 May 2013.
    http://www.cecam.org/workshop-930.html
15. Organizer of the CFCAM workshop 'Pseudopotentials and PAW atomic data: beyond a "black art"?'
    Paris (France), 28-29 January 2014

6. Grants and research contracts

– Firmin Van Brée Fellowship 1998-99 of the Hoover Foundation of the Belgian American Educational Foundation
– Grantee of the Fulbright Program 1998-99 of the Commission for Educational exchange
– Principal Investigator of the project "Etude ab initio des propriétés structurales et électroniques de diverses interfaces métal/high−k dans le cadre de la miniaturisation des transistors MOS", Fonds Spéciaux de Recherche de l'UCL, 2004 (55 k€)
– Principal Investigator of the project "Etude ab initio des propriétés structurales et électroniques de diverses interfaces métal/high−k dans le cadre de la miniaturisation des transistors MOS.", Crédit aux chercheurs du FNRS, exercice 2004-2005 (32 k€)
– Staff member in the project "Nanoscale Quantum Simulations for Nanostructures and Advanced Materials (NANOQUANTA)", Network of Excellence funded by the EU FP6, 1 June 2004 - 31 May 2008 (Total: 5000 k€ ; UCL share: 450 k€). [contract n° NMP4-CT-2004-500198]
– Staff member in the project "Quantum effects in clusters and nanowires", Pôle d'Attraction Interuniversitaire PAI/UIAPP (UCL-KUL-UA-UH-ULg) phase VI, 1 January 2007- 31 December 2011 (Total: 5000 k€ ; UCL share : 1200 k€).
– co-Principal Investigator of the project "Nanosytèmes hybrides métal/organique", Action de Recherche Concertée de la Communauté Française de Belgique, 1 September 2007 - 31 August 2012 (Total: 1000 k€ shared between 6 promotors)
– co-Principal Investigator of the project "Imagerie et contrôle du transport de charge dans des nanodispositifs" (Fonds de la Recherche Fondamentale Collective du FRS-FNRS, 1 January 2008 - 31 December 2011 (220 k€ de frais d'équipement et 120 k€ de frais de fonctionnement) [contract nº FRFC 2.4546.08]
– Principal Investigator of the research project "High-k dielectrics" between IMEC and UCL: 1 October 2008 - 31 September 2013 (140 k€)
– co-Principal Investigator of the project "Imagerie et contrôle du transport de charge dans des nanodispositifs", Fonds Spéciaux de Recherche de l'UCL, 2008 (90 k€)
– Staff member in the project "European Theoretical Spectroscopy Facility (ETSF)", Integrated Infrastructure Initiative funded by the EU FP7, 1 January 2008 - 30 Juin 2011 (Total amount 3800 k€, shared between 11 nodes).
– co-Principal Investigator of the project "In Silico Materials Design and experimental validation for novel optical coatings (ISIMADE)", Strategisch Basis Onderzoek (SBO) funded by the IWT Vlaanderen, 1 January 2009 - 31 December 2012 (Total: 1800 k€ ; UCL share: 315 k€).
– co-Principal Investigator of the project "Cellules solaires photovoltaïques à base CZTS" funded by the Walloon Region (Plan Marshall, Pôle Mecatech), 1 November 2012 - 31 October 2016 (Total: 3500 k€ ; share: 160 k€)
– Principal Investigator of the project "Etude ab initio des propriétés structurales, thermodynamiques, électroniques, et optiques du CZTS dans le cadre des cellules photovoltaïques de 2ème génération", Fonds Spéciaux de Recherche de l'UCL 2013, 1 January 2013-31 December 2015 (49.5 k€).
– co-Principal Investigator of the project "Materials Project" in collaboration with the Lawrence Berkeley National Laboratory (Berkeley, California, USA), Fonds d'appui à l'internationalisation de l'UCL, 2013 (15 k€).
– co-Principal Investigator of the project "Vibrational Spectroscopy: a Combined Theoretical and Experimental Approach"of the MIT-Belgium UCL Seed Funds,, 1 March 2014-31August 2015- (25k$).
– co-Principal Investigator of the project "BATWAL (Phase 1): Développement de batteries lithium-ion à peindre pour le stockage local et leur intégration dans le réseau global pour une gestion efficace de l'énergie électrique en Wallonie" funded by the Walloon Region (Programmes d'excellence): 1 March 2014-31 Juillet 2016 (Total: 2570 k€ - UCL share: 1000 k€)

7. Short-term stays abroad

– **22 March 2013-28 March 2013**: one-week stay at the Massachusetts Institute of Technology (MIT), Cambridge MA (USA), as Visiting Professor in the groups of Profs. G. Ceder, J. Grossman, and J. Li in the framework of the MIT International Science and Technology Initiatives (MISTI).

– **16 April 2012-30 April 2012**: two-week stay at the Institute of Physics and at Institute of Computational Mathematics, Chinese Academy of Sciences (CAS), Beijing (China), as Visiting Professor in the groups of Profs. Z. Fang, X. Dai, and A. Zhou.

– **15 November 2011-23 November 2011**: one-week stay at the Institute of Computational Mathematics, Chinese Academy of Sciences (CAS), Beijing (China), as Visiting Professor in the group of Prof. A. Zhou.

– **22 June 2011-10 July 2011**: two-week stay the Università di Cagliari, Cagliari (Italy), as Visiting Professor in the group of Prof. G. Cappellini.

– **15 November 2010-29 November 2010**: two-week stay at the Institute of Computational Mathematics, Chinese Academy of Sciences (CAS), Beijing (China), as Visiting Professor in the group of Prof. A. Zhou, in the framework of the CAS-FNRS collaboration program.

– **15 November 2009-5 December 2009**: three-week stay at the Kavli Institute for Theoretical Physics, Santa Barbara CA (USA), as a Invited Professor to the program "Excitations in Condensed Matter: From Basic Concepts to Real Materials".

– **16 June 2007-23 June 2007**: one-week stay at the Universtité de Montréal, Montréal (Canada), as a Visiting Scientist in the group of Prof. M. Côté.

– **15 May 2004-18 June 2004**: five-week stay at the Université Claude Bernard – Lyon 1, Lyon (France), as Invited Professor in the group of Dr. X. Blase (Laboratoire de Physique de la Matière et des Nanostructures).

– **21 April 2000-28 April 2000**: one-week stay at the Ecole Polytechnique Fédérale de Lausanne, Lausanne (Switzerland), as Visiting Scientist in the IRRMA group of Prof. A. Pasquarello.

– **16 January 2000-30 January 2000**: two-week stay at the University of California at Berkeley, Berkeley CA (USA), as Holder of a 'Bourse scientifique pour bref séjour à l'étranger 2000' of the FNRS-Belgium, in the group of Prof. S. G. Louie.

– **18 September 1998-2 October 1998**: two-week stay at the Université de Paris Sud, Orsay (France), as a Visiting Scientist in the group of Prof. C. Noguera (Laboratoire de Physique des Solides).

– **15 August 1998-12 September 1998**: four-week stay at the University of California at Berkeley, Berkeley CA (USA), as Holder of a 'Bourse scientifique pour bref séjour à l'étranger 1998' of the FNRS-Belgium, in the group of Prof. S. G. Louie.

– **21 April 1997-2 May 1997**: two-week stay at the Ecole Polytechnique Fédérale de Lausanne, Lausanne (Switzerland), as scientific guest in the IRRMA group of Prof. R. Car.

– **1 August 1996-1 January 1997**: five-month stay at the Ecole Polytechnique Fédérale de Lausanne, Lausanne (Switzerland), as Software Development Consultant for the PATP, in the IRRMA group of Prof. R. Car.

– **7 April 1996-7 July 1996**: three-month stay at the Ecole Polytechnique Fédérale de Lausanne, Lausanne (Switzerland), as Award Winner of the 'Concours des Bourses de Voyages 1996' of the 'Communauté Française de Belgique', in the IRRMA group of Prof. R. Car.

– **9 August 1993-10 September 1993**: five-week stay at the Massachusetts Institute of Technology (MIT), Cambridge MA (USA), as Summer Student in the group of Prof. M. S. Dresselhaus.

8. Most significant publications

1. Nitrogen Incorporation at Si(001)/SiO_2 Interfaces:
   Relation between N *1s* Core-Level Shifts and Microscopic Structure
   G.-M. Rignanese, A. Pasquarello, J.-C. Charlier, X. Gonze, and R. Car
   Phys. Rev. Lett. **79**, 5174-5177 (1997)

2. Quasiparticle effects on tunneling currents: a study of C_2H_4 adsorbed on the Si(001)-2×1 surface
   G.-M. Rignanese, X. Blase, and S. G. Louie
   Phys. Rev. Lett. **86**, 2110-2113 (2001)

3. Electronic structure of carbon nanocones
   J.-C. Charlier and G.-M. Rignanese
   Phys. Rev. Lett. **86**, 5970-5973 (2001)

4. First-principles study of dynamical and dielectric properties of tetragonal zirconia
   G.-M. Rignanese, F. Detraux, X. Gonze, and A. Pasquarello
   Phys. Rev. B **64**, 134301:1-7 (2001)

5. Dielectric constants of Zr silicates: A first-principles study
   G.-M. Rignanese, F. Detraux, X. Gonze, A. Bongiorno, and A. Pasquarello
   Phys. Rev. Lett. **89**, 117601:1-4 (2002)

6. First-principles computation of material properties : the ABINIT software project
   X. Gonze, J.-M. Beuken, R. Caracas, F. Detraux, M. Fuchs, G.-M. Rignanese, L. Sindic, M. Verstraete, G. Zerah, F. Jollet, M. Torrent, A. Roy, M. Mikami, P. Ghosez, J.-Y. Raty, and D.C. Allan
   Comp. Mater. Sci. **25**, 478-492 (2002)

7. First-principles investigation of high-κ dielectrics: Comparison between the silicates and oxides of hafnium and zirconium
   G.-M. Rignanese, X. Gonze, G. Jun, K. Cho, and A. Pasquarello
   Phys. Rev. B **69**, 184301:1-10 (2004)

8. Room temperature Peierls distortion in small diameter nanotubes
   D. Connétable, G.-M. Rignanese, J.-C. Charlier, and X. Blase
   Phys. Rev. Lett. **94**, 015503:1-4 (2005)

9. A brief introduction the ABINIT software package
   X. Gonze, G.-M. Rignanese, M. Verstraete, J.-M. Beuken, Y. Pouillon, R. Caracas, F. Jollet, M. Torrent, G. Zerah, M. Mikami, P. Ghosez, M. Veithen, J.-Y. Raty, V. Olevano, F. Bruneval, L. Reining, R. Godby, G. Onida, D. R. Hamann, and D. C. Allan
   Z. Kristallogr. **220**, 558-562 (2005)

10. Band Offsets at the Si/SiO_2 Interface from Many-Body Perturbation Theory
    R. Shaltaf, G.-M. Rignanese, X. Gonze, F. Giustino, and A. Pasquarello
    Phys. Rev. Lett. 100, 186401:1-4 (2008)

9. Complete list of publications

A. Journal articles

1. Scaling hypothesis for corrections to total energy and stress in plane-wave based ab initio calculations
   G.-M. Rignanese, P. Ghosez, J.-C. Charlier, J.-P. Michenaud, and X. Gonze
   Phys. Rev. B **5**2, 8160-8178 (1995)

2. Ab initio study of the volume dependence of dynamical and thermodynamical properties of silicon
   G.-M. Rignanese, J.-P. Michenaud, and X. Gonze
   Phys. Rev. B **53**, 4488-4497 (1996)

3. Nitrogen Incorporation at Si(001)/SiO_2 Interfaces:
   Relation between N *1s* Core-Level Shifts and Microscopic Structure
   G.-M. Rignanese, A. Pasquarello, J.-C. Charlier, X. Gonze, and R. Car
   Phys. Rev. Lett. **79**, 5174-5177 (1997)

4. Theoretical modeling of the nucleation and growth of Aluminium films thermally
   evaporated onto Poly (ethylene terephthalate) substrate
   Y. Travaly, P. Bertrand, G.-M. Rignanese, and X. Gonze
   J. Adhesion **66**, 339-355 (1998)

5. First-principles study of NH_3 exposed Si(001)-2×1:
   Relation between N *1s* core-level shifts and atomic structure
   G.-M. Rignanese and A. Pasquarello
   Appl. Phys. Lett. **76**, 553-555 (2000)

6. First-Principles Molecular Dynamics Study of the (0001) α-Quartz Surface
   G.-M. Rignanese, A. De Vita, J.-C. Charlier, X. Gonze, and R. Car
   Phys. Rev. B **61**, 13250-13255 (2000)

7. Glutathione Transferase: A First-Principles Study of the Active Site
   G.-M. Rignanese, F. De Angelis, S. Melchionna, and A. De Vita
   J. Am. Chem. Soc. **122**, 11963-11970 (2000)

8. Nitrogen bonding configurations at nitrided Si(001) surfaces and Si(001)-SiO_2 interfaces:
   a first-principles study of core-level shifts
   G.-M. Rignanese and A. Pasquarello
   Phys. Rev. B **63**, 075307:1-10 (2001)

9. First-principles study of structural, electronic, dynamical, and dielectric properties of zircon
   G.-M. Rignanese, X. Gonze, and A. Pasquarello
   Phys. Rev. B **63**, 104305:1-7 (2001)

10. Quasiparticle effects on tunneling currents: a study of C_2H_4 adsorbed on the Si(001)-2×1 surface
    G.-M. Rignanese, X. Blase, and S. G. Louie
    Phys. Rev. Lett. **86**, 2110-2113 (2001)

11. First-principles study of dynamical and dielectric properties of tetragonal zirconia
    G.-M. Rignanese, F. Detraux, X. Gonze, and A. Pasquarello
    Phys. Rev. B **64**, 134301:1-7 (2001)

12. Nitrogen *1s* core-level shifts at the NH_3 saturated Si(100)-2×1 surface: a first-principles study
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G.-M. Rignanese
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27. La liaison hydrogène dans des systèmes biologiques: comparaison de plusieurs codes
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GDR 'Fonctionnelle de la densité: de la molécule aux matériaux et systèmes complexes'
Dinard (France), 22-24 May 2002.

28. The self-assembly and the hydrogen bond in biological and bio-inorganic systems
X. Rocquefelte, G.-M. Rignanese, J.-C. Charlier, X. Gonze, P. Koenig, and M. Elstner
COMELCAN Meeting 2002
San Sebastián (Spain), 3-5 June 2002.

29. The ABINIT software project (invited talk)
X. Gonze, G.-M. Rignanese, and G. Zerah
CECAM Workshop on Open Source Software for Microscopic Calculations
Lyon (France), 19-21 June 2002.

30. Hydration and dehydration of various quartz surfaces: a first-principles study (invited talk)
G.-M. Rignanese, J.-C. Charlier, and X. Gonze
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31. Calculating *GW* corrections with ABINIT
V. Olevano, R. Godby, L. Reining, G. Onida, M. Torrent, and *G.-M. Rignanese*
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Louvain-la-Neuve (Belgium), 6-8 November 2002.

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Velen (Germany), 19-23 September 2003.

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G.-M. Rignanese
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Montréal (Canada), 22-26 March 2004.
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G.-M. Rignanese
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Lyon (France), 13-15 September 2004.

38. First-principles study of crystalline and amorphous transition metal oxides and silicates
G.-M. Rignanese, F. Detraux, X. Rocquefelte, J. Bouchet, X. Gonze, A. Bongiorno, F. Giustino, and A. Pasquarello
Workshop on Theory and Modeling of Electronic Excitations in Nanoscience (NANOEXC'04)
Acquafredda di Maratea (Italy), 19-23 September 2004.

39. Density-functional perturbation theory, and its applications in mineral sciences (invited talk)
X. Gonze, G.-M. Rignanese, and R. Caracas
CECAM Workshop on First-Principles Simulations: Perspectives and Challenges in Mineral Sciences
Lyon (France), 27 September-1 October 2004.

40. New Materials for Nano-electronics: A First-Principles Study (invited talk)
G.-M. Rignanese
Third scientific meeting of the Wallonia Network for Nanotechnologies (NANOWAL)
Mons (Belgium), 22 April 2005.

41. Electronic and dielectric properties of group IVB transition metal oxides (invited talk)
G.-M. Rignanese
EMRS Spring Meeting 2006
Nice (France), 29 May- 2 June 2006.

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G.-M. Rignanese
International Symposium on Structure-Property Relationships in Solid State Materials
Bordeaux (France), 27-30 June 2006.

43. First-Principles Calculations of Band Offsets of SiO_2 and $ZrSiO_4$ with Silicon
R. Shaltaf, J. Bouchet, G.-M. Rignanese, X. Gonze, F. Bruneval, L. Reining, F. Giustino, and A. Pasquarello
11th Nanoquanta Workshop on Electronic Excitations: A decade of applications of the Bethe-Salpeter Equation
Houffalize (Belgium), 19-22 September 2006.

44. Electronic and dielectric properties of group IVB transition metal oxides (invited talk)
G.-M. Rignanese
212th Electrochemical Society Meeting
Washington DC (USA), 7-12 October 2007.

45. First-Principles Investigation of High-K Dielectrics (invited talk)
G.-M. Rignanese
Workshop "Oxydes fonctionnels pour l'intégration en micro- et nano-électronique"
Autrans (France), 16-19 March 2008.

46. *GW* and hybrid functional corrections to the calculation of transport properties in organic systems
A. Ferretti, P.E. Trevisanutto, V. Olevano, L. Martin-Samos, A. Ruini, T. Rangel, and G.-M. Rignanese
13th Nanoquanta/ETSF Conference on Electronic Excitations
Pugnochiuso-Vieste (Italy), 23-27 September 2008.

47. Electronic Transport in zig-zag Graphene Nanoribbons
S. M.-M. Dubois, G.-M. Rignanese, and J.-C. Charlier
13th Nanoquanta/ETSF Conference on Electronic Excitations
Pugnochiuso-Vieste (Italy), 23-27 September 2008.

48. Band offsets from Many-Body Perturbation Theory (invited talk)
G.-M. Rignanese
14th International Workshop on Computational Condensed-Matter Physics
International Center for Theoretical Physics, Trieste (Italy), 8-10 January 2009.

49. A Many-Body Perturbation Theory perspective to defects in microelectronic devices and materials
G.-M. Rignanese (invited talk)
CECAM Workshop "Which Electronic Structure Method for the Study of Defects?"
Lausanne (Switzerland), 8-10 June 2009.

50. Band offsets calculations: from Density Functional Theory to Many-Body Perturbation Theory
G.-M. Rignanese (invited talk)
Workshop "Theory and Modelling of Quantum Confined Materials"
ISEN, Lille (France), 10-11 June 2009

51. Oxidize this: A study of PAW+QPSCGW calculations on Zn and Sn oxides
*M. Stankovsk*i, A. Miglio, G. Geadah-Antonius, M. Giantomassi, G.-M. Rignanese, and X. Gonze
14th ETSF Conference on Electronic Excitations
Evora (Portugal), 14-19 September 2009.

52. Quantum Transport in Graphene Nanoribbons (invited talk)
S. M.-M. Dubois, G.-M. Rignanese, and J.-C. Charlier
14th ETSF Conference on Electronic Excitations
Evora (Portugal), 14-19 September 2009.

53. Calcul des décalages de bandes aux interfaces: de la DFT à l'approximation GW (invited talk)
G.-M. Rignanese
Workshop "Développements et Applications de Méthodes de Simulation pour la Modélisation des Matériaux"
Lyon (France), 28-30 September 2009.

54. *GW* method and PAW formalism applied to ZnO and SnO
G. Antonius, *M. Stankovski*, A. Miglio, G.-M. Rignanese, and M. Côté
2010 March meeting of the American Physical Society
Portland OR (USA), 15-19 March 2010.

55. Transport properties of molecular junctions from Many-Body Perturbation Theory (invited talk)
T. Rangel, A. Ferretti, P.E. Trevisanutto, V. Olevano, and G.-M. Rignanese
15th ETSF Conference on Electronic Excitations
Berlin (Germany), 12-15 October 2010.

56. What is the G_0W_0 band-gap of ZnO (invited talk)
G.-M. Rignanese, M. Stankovski, G. Antonius, D. Waroquiers, A. Miglio, H. Dixit, P. Rinke, H. Jiang, M. Giantomassi, X. Gonze, and M. Côté
CECAM Workshop "Challenges and Solutions in *GW* Calculations for Complex Systems"
Lausanne (Switzerland), 7-10 June 2011.

57. The G_0W_0 band-gap of ZnO: effects of plasmon-pole models (invited talk)
M. Stankovski, G. Antonius, A. Miglio, D. Waroquiers, M. Côté, X. Gonze, and G.-M. Rignanese
16th ETSF Conference on Electronic Excitations
Torino (Italy), 27-30 September 2011.

58. Current issues in the description of charged defects: the case of hydrogen in amorphous silica
D. Waroquiers, M. Giantomassi, M. Stankovski, G.-M. Rignanese, and X. Gonze
16th ETSF Conference on Electronic Excitations
Torino (Italy), 27-30 September 2011.

59. The ABINIT software project (invited talk)
G.-M. Rignanese
2011 One-day Workshop on Optimization in Materials Computing
Beijing (China), 16 November 2011.

60. Assessment of electronic band structure from the Tran-Blaha functional:
comparison with Many-Body Perturbation Theory resuls
D. Waroquiers, A. Lherbier, A. Miglio, M. Stankovski, S. Poncé, M. Oliveira, M. Giantomassi, G.-M. Rignanese, and X. Gonze
17th ETSF Conference on Electronic Excitations
Coimbra (Portugal), 2-5 October 2012.

61. High-throughput ab initio computations for materials discovery and the Materials Project database
G. Hautier, A. Miglio, G.-M. Rignanese, X. Gonze, A. Jain, K. Persson, S. Ping Ong, and G. Ceder,
17th ETSF Conference on Electronic Excitations
Coimbra (Portugal), 2-5 October 2012.

62. A High-Throughput Computational Search for New Transparent Conducting Oxides
G. Hautier, A. Miglio, G. Ceder, G.-M. Rignanese, and X. Gonze,
2013 March meeting of the American Physical Society.
Baltimore MD (USA), 17-22 March 2013.

63. Reliability of the Tran-Blaha functional in predicting band gaps and widths
G.-M. Rignanese, D. Waroquiers, A. Lherbier, A. Miglio, M. Stankovski, S. Poncé, M. Oliveira, M. Giantomassi, and X. Gonze
2013 March meeting of the American Physical Society.
Baltimore MD (USA), 17-22 March 2013.

64. Accuracy of Generalized Gradient Approximation functionals
for density functional perturbation theory calculations (invited talk)
L. He, F. Liu, G. Hautier, M.J.T. Oliveira, M.A.L. Marques, F.D. Vila, J.J. Rehr, G.-M. Rignanese, and A. Zhou
6th International ABINIT Developer Workshop
Dinard (France), 15-18 April 2013.

65. Towards high-throughput ab initio calculations using ABINIT.
G. Antonius, M. Côté, M. Giantomassi, X. Gonze, G. Hautier, *G.-M. Rignanese*, M. Stankovski, and D. Waroquiers
6th International ABINIT Developer Workshop
Dinard (France), 15-18 April 2013.

66. Accelerating materials discovery with *ab initio* methods
through high-throughput and data mining (invited talk)
G.-M. Rignanese, G. Hautier, A. Miglio, X. Gonze, and G. Ceder
GDR 'Code Développement Formalisme (CoDFT): Des approches semi-empiriques à la Théorie de la Fonctionnelle de la Densité et au-delà'
Guidel-les-Bains (France), 21-24 May 2013.

67. Identification and design of novel p-type transparent conducting oxides through high-throughput computing
G. Hautier, A. Miglio, G. Ceder, G.-M. Rignanese, and X. Gonze,
EMRS Spring Meeting 2013.
Strasbourg (France), 27-31 May 2013.

68. Materials design through high-throughput ab initio computing and data mining (invited talk)
G.-M. Rignanese, G. Hautier, A. Miglio, X. Gonze, and G. Ceder
Minisymposium: Trends in *GW*-approaches for Nano-Sciences in Europe
Karlsruhe (Germany), 25-26 July 2013.

69. Finding low hole effective masses p-type transparent conducting oxides through high-throughput computing
G. Hautier, A. Miglio, G. Ceder, G.-M. Rignanese, and X. Gonze,
European Congress and Exhibition on Advanced Materials and Processes (EUROMAT) 2013
Sevilla (Spain), 8-13 September 2013.

70. Identification of Low Hole Effective Mass Novel p-type Transparent Conducting Oxides by high-throughput computing
G. Hautier, A. Miglio, J. Varley, G. Ceder, G.-M. Rignanese, and X. Gonze,
18th ETSF Conference on Electronic Excitations
Luxembourg (Luxembourg), 1-4 October 2013.

71. Towards a better error assessment of first-principles methods for electronic and optical properties of solids
G.-M. Rignanese (invited talk)
International workshop on computational physics and materials science, "Total energy and force methods"
Lausanne (Switzerland), 9-11 january 2014.

72. Abinit contribution to the Materials Project (invited talk)
G.-M. Rignanese
SIXNS-III Workshop "Theoretical software and analysis tools and software integration for scattering science"
Seattle WA (USA), 17-18 january 2014.

73. Accelerating materials discovery with ab initio methods through high-throughput and data mining
G.-M. Rignanese (invited talk)
QuantumHagen: Modeling of Electronic Devices and Materials at the Nanoscale
Copenhagen (Denmark), 1-3 july 2014.

11. Seminars

1. Parallélisation d'un programme de calcul de propriétés des matériaux
   X. Gonze and G.-M. Rignanese
   Local Scalable Computing Working Group. Louvain-la-Neuve (Belgium), 2 June 1994.
2. Simulation des solides au niveau microscopique
   X. Gonze and G.-M. Rignanese
   Local Scalable Computing Working Group. Louvain-la-Neuve (Belgium), 24 May 1995.
3. SiO_2: its surface and its interface with Si
   G.-M. Rignanese
   Université Catholique de Louvain, Louvain-la-Neuve (Belgium), 10 March 1997.
4. Etude du SiO_2 par Dynamique Moléculaire Ab Initio: surface et interface avec le Si
   G.-M. Rignanese
   Laboratoire de Physique des Solides, Université de Paris Sud, Orsay (France), 24 September 1998.
5. Quasiparticle band structure of C_2H_4 adsorbed on the Si(001)-2×1 surface within the *GW* approximation
   G.-M. Rignanese
   Institut d'Electronique et de Microélectronique du Nord, Lille (France), 22 June 2000.
6. Oxides de grille alternatifs: l'apport du calcul ab initio
   G.-M. Rignanese, F. Detraux, and X. Gonze
   1st Feynman Workshop of the Research Center in Micro and Nanoscopic Materials and Electronic Devices
   Université Catholique de Louvain, Louvain-la-Neuve (Belgium), 2 May 2001.
7. Activités de recherches actuelles et projets futures
   G.-M. Rignanese
   Département de Chimie de l'Université de Liège, Liège (Belgium), 17 April 2002.
8. Etude *ab initio* des constantes diélectriques de silicates de zirconium $(ZrO_2)_x(SiO_2)_{1-x}$
   G.-M. Rignanese
   2nd Feynman Workshop of the Research Center in Micro and Nanoscopic Materials and Electronic Devices
   Université Catholique de Louvain, Louvain-la-Neuve (Belgium), 22 May 2002.
9. Physical Properties from Density Functional Theory
   G.-M. Rignanese and X. Gonze
   IMEC (Interuniversity MicroElectronics Center), Leuven (Belgium), 31 January 2003.
10. Dielectric constants of Zr and Hf oxides and silicates: A first-principles study
    G.-M. Rignanese
    IMEC (Interuniversity MicroElectronics Center), Leuven (Belgium), 31 January 2003.
11. Transition metal oxides and silicates as high-κ dielectrics: a first-principles investigation
    G.-M. Rignanese
    Teleconference with Philips Research Leuven and Motoral Inc. (Phoenix and Austin)
    Philips Research Leuven, Leuven (Belgium), 23 May 2003.
12. Le calcul ab initio: un soutien théorique aux expérimentateurs
    G.-M. Rignanese
    3rd Feynman Workshop of the Research Center in Micro and Nanoscopic Materials and Electronic Devices
    Université Catholique de Louvain, Louvain-la-Neuve (Belgium), 15 September 2003.
13. Group IVB transition metal oxides and silicates as high-κ dielectrics: A first-principles study
    G.-M. Rignanese
    Institut Romand de Recherche Numérique en Physique des Matériaux (IRRMA),
    Ecole Polytechnique Fédérale de Lausanne, Lausanne (Switzerland), 17 October 2003.
14. Etude ab initio des oxides et silicates cristallins et amorphes de métaux de transition
    G.-M. Rignanese
    Laboratoire de Physique de la Matière et des Nanostructures (LPMCN)
    Université Claude Bernard – Lyon 1, Lyon (France), 29 October 2004.

15. Quasiparticle band offsets at various interfaces
    G.-M. Rignanese
    Institut Romand de Recherche Numérique en Physique des Matériaux (IRRMA),
    Ecole Polytechnique Fédérale de Lausanne, Lausanne (Switzerland), 30 November 2004.

16. First-principles investigation of high-k dielectrics
    G.-M. Rignanese
    Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin (Germany), 28 April 2005.

17. Band Offsets Predictions using Quasiparticle Calculations
    R. Shaltaf and G.-M. Rignanese
    IMEC (Interuniversity MicroElectronics Center), Leuven (Belgium), 8 February 2006.

18. Electronic and dielectric properties of group IVb transition metal oxides
    G.-M. Rignanese
    Université de Montréal, Montréal (Canada), 18 June 2007.

19. Band Offsets at the Si/SiO_2 Interface from Many-Body Perturbation Theory
    G.-M. Rignanese
    Ecole Polytechnique Fédérale de Lausanne, Lausanne (Switzerland), 14 May 2008.

20. First-Principles Investigation of High-K Dielectrics
    G.-M. Rignanese
    Institut Néel, CNRS et Université Joseph Fourier, Grenoble (France), 19 June 2008.

21. Quantum Transport at UCLouvain
    G.-M. Rignanese
    University of York, York (United Kingdom),11 July 2008.

22. The Green Projetct
    G.-M. Rignanese
    Université Catholique de Louvain, Louvain-la-Neuve (Belgium), 31 October 2008.

23. Transport électronique quantique:l'état des recherches menées à l'UCLouvain
    G.-M. Rignanese
    Institut Néel, CNRS et Université Joseph Fourier, Grenoble (France), 3 December 2008.

24. Band offsets at the Si/SiO_2 interface from Many-Body Perturbation Theory
    G.-M. Rignanese
    IMEC (Interuniversity MicroElectronics Center), Leuven (Belgium), 10 December 2008.

25. Vibrational spectroscopy
    G.-M. Rignanese
    Kavli Institute for Theoretical Physics, Santa Barbara CA (USA), 20 November 2009.

26. Electronic structure calculations: from Density Functional Theory to Many-Body Perturbation Theory
    G.-M. Rignanese
    Institute of Computational Mathematics and Scientific/Engineering Computing (ICMSEC),
    Chinese Academy of Sciences (CAS), Beijing (China), 19 November 2010.

27. Band-offsets from Many-Body Perturbation Theory
    G.-M. Rignanese
    College of Chemistry, Peking University, Beijing (China), 22 November 2010.

28. The ABINIT software project
    G.-M. Rignanese
    Supercomputing Center of the Chinese Academy of Sciences, Beijing (China), 26 November 2010.

29. Transport properties of molecular junctions from many-body perturbation theory
    G.-M. Rignanese
    University of York, York (United Kingdom), 5 April 2011.

30. From micro to molecular electronics: a first-principles approach
    G.-M. Rignanese
    Institute of Computational Mathematics and Scientific/Engineering Computing (ICMSEC),
    Chinese Academy of Sciences (CAS), Beijing (China), 18 November 2011.

31. The Materials Project: Accelerating materials discovery with ab initio methods through high-throughput and data mining
    G.-M. Rignanese
    Institute of Computational Mathematics and Scientific/Engineering Computing (ICMSEC),
    Chinese Academy of Sciences (CAS), Beijing (China), 20 April 2012.

32. From micro to molecular electronics: a first-principles approach
    G.-M. Rignanese
    Institute of Physics (IOP),
    Chinese Academy of Sciences (CAS), Beijing (China), 25 April 2012.

33. Accelerating materials discovery with ab initio methods through high-throughput and data mining
    G.-M. Rignanese
    Peter Grünberg Institute and Institute for Advanced Simulation
    Forschungszentrum Jülich, Jülich (Germany), 16 October 2013.

34. Accelerating materials discovery with ab initio methods through high-throughput and data mining
    G.-M. Rignanese
    Materials Department, University of Oxford, Oxford (United Kingdom), 31 October 2013.

12. Invited lectures

1. Spectroscopies
   G.-M. Rignanese
   CECAM Tutorial "Electronic Excitations and Spectroscopies: Theory and Codes"
   Lyon (France), 11-15 december 2006.
2. Calculs théoriques de la structure électronique des solides
   G.-M. Rignanese
   Facultés Universitaires Notre-Dame de la Paix. Namur (Belgium), 4 December 2007.
3. Spectroscopies
   G.-M. Rignanese
   CECAM Tutorial "Electronic Excitations and Spectroscopies: Theory and Codes"
   Lyon (France), 10-14 december 2007.
4. Spectroscopies
   G.-M. Rignanese
   CECAM Tutorial "Electronic Excitations and Spectroscopies: Theory and Codes"
   Zurich (Switzerland), 24-29 May 2009.
5. Linear responses to atomic displacements and static electric fields
   G.-M. Rignanese
   CECAM Tutorial "Linear and non-linear responses of solids with the ABINIT software : phonons, electric fields, and other perturbations"
   Lausanne (Switzerland), 26-30 April 2010.
6. Symmetries of phonons
   G.-M. Rignanese
   CECAM Tutorial "Linear and non-linear responses of solids with the ABINIT software : phonons, electric fields, and other perturbations"
   Lausanne (Switzerland), 26-30 April 2010.
7. First-principles electronic structure calculations: from Density Functional Theory to Many-Body Perturbation Theory
   G-M. Rignanese
   School on "Computational Modelling of Materials", Universiteit Antwerpen (Belgium), 2 December 2010.
8. First-principles calculations of materials for electronics
   G-M. Rignanese
   School on "Computational Modelling of Materials", Universiteit Antwerpen (Belgium), 2 December 2010.
9. Introduction to Many-Body Perturbation Theory and the GW approximation
   G.-M. Rignanese
   CECAM Tutorial "Theoretical Spectroscopy Lectures"
   Lausanne (Switzerland), 1-5 May 2011.
10. Theoretical Spectroscopy Methods in Condensed Matter Physics
    G.-M. Rignanese
    Università di Cagliari, Cagliari (Italy), 23, 24, 30 June, and 4 July 2011.
11. Density-functional theory in the ABINIT code
    G.-M. Rignanese
    International summer school on New trends in computational approaches for many-body systems
    Sherbrooke, Québec (Canada), 28 May to 8 June 2012.
12. Many-Body Perturbation Theory: the *GW* method
    G.-M. Rignanese
    International summer school on New trends in computational approaches for many-body systems
    Sherbrooke, Québec (Canada), 28 May to 8 June 2012.

13. Linear responses to atomic displacements and static electric fields
    G.-M. Rignanese
    CECAM Tutorial “Response treatment for the dynamical properties of materials with the ABINIT package”
    Zurich (Switzerland), 22-26 October 2012.

14. Symmetries of phonons
    G.-M. Rignanese
    CECAM Tutorial “Response treatment for the dynamical properties of materials with the ABINIT package”
    Zurich (Switzerland), 22-26 October 2012.

15. Density Functional Theory
    G.-M. Rignanese
    CECAM Tutorial “Theoretical Spectroscopy Lectures”
    Lausanne (Switzerland), 13-17 May 2013.

16. Linear responses to atomic displacements and static electric fields
    G.-M. Rignanese
    CECAM Tutorial “Dynamical, dielectric and magnetic properties of solids with ABINIT”
    Lyon (France), 12-16 May 2014.

17. Symmetries of phonons
    G.-M. Rignanese
    CECAM Tutorial “Dynamical, dielectric and magnetic properties of solids with ABINIT”
    Lyon (France), 12-16 May 2014.

18. Density-functional theory in the ABINIT code
    G.-M. Rignanese
    International summer school on Computational Methods for Quantum Materials
    Sherbrooke, Québec (Canada), 26 May to 6 June 20124.

19. Many-Body Perturbation Theory: the GW method
    G.-M. Rignanese
    International summer school on Computational Methods for Quantum Materials
    Sherbrooke, Québec (Canada), 26 May to 6 June 20124.

13. Posters at professional meetings

1. Corrections to total energy and stress in plane-wave based ab initio calculations
   G.-M. Rignanese, Ph. Ghosez, J.-C. Charlier, J.-P. Michenaud, and X. Gonze

   – 7th International Workshop on Computational Condensed-Matter Physics
     International Center for Theoretical Physics, Trieste (Italy), 11-15 January 1995.
   – 1995 March meeting of the American Physical Society
     San José CA (USA), 20-24 March 1995.
   – 7th Annual Workshop on Recent Developments in Electronic Structure Algorithms
     St. Mary's City MD (USA), 19-22 May 1995.

   Abstract in Bull. Am. Phys. Soc. **40**, 367 (1995).

4. Parallel computation of ab initio dynamical matrices
   G.-M. Rignanese, J.-M. Beuken, J.-P. Michenaud, and X. Gonze

   – 7th International Workshop on Computational Condensed-Matter Physics
     International Center for Theoretical Physics, Trieste (Italy), 11-15 January 1995.
   – 1995 March meeting of the American Physical Society
     San José CA (USA), 20-24 March 1995.

   Abstract in Bull. Am. Phys. Soc. **40**, 177 (1995).

6. Ab initio study of the volume dependence of dynamical and thermodynamical properties of silicon
   G.-M. Rignanese, J.-P. Michenaud, and X. Gonze

   – 1996 March meeting of the American Physical Society
     St Louis MO (USA), 18-22 March 1996.
   – 15th General Conference of Condensed-Matter Division of the European Physical Society
     Baveno-Stresa (Italy), 22-25 April 1996.

   Abstract in Bull. Am. Phys. Soc. **41**, 338 (1996).

8. Ab initio study of SiO_2 (α-quartz) surface
   G.-M. Rignanese, J.-P. Michenaud, X. Gonze, and Ph. Lambin
   15th General Conference of Condensed-Matter Division of the European Physical Society
   Baveno-Stresa (Italy), April 22-25, 1996.

9. Nitrogen Incorporation at the Si(001)/SiO_2 Interface: a First-Principles Study
   G.-M. Rignanese, A. Pasquarello, J.-C. Charlier, X. Gonze and R. Car
   8th International Workshop on Computational Condensed-Matter Physics
   International Center for Theoretical Physics, Trieste (Italy), 9-11 January 1997.

10. First Principles Study of the (0001) α-Quartz surface
    G.-M. Rignanese, J.-P. Michenaud, X. Gonze, X. Blase, J.-C. Charlier, A. De Vita, and R. Car

    – 8th International Workshop on Computational Condensed-Matter Physics
      International Center for Theoretical Physics, Trieste (Italy), 9-11 January 1997.
    – 16th General Conference of Condensed-Matter Division of the European Physical Society
      Leuven (Belgium), 25-28 August 1997.

12. The Aluminium/Poly (ethylene terephthalate) interface: A density functional theory study
    Y. Travaly, P. Bertrand, X. Gonze, and G.-M. Rignanese
    8th International Workshop on Computational Condensed-Matter Physics
    International Center for Theoretical Physics, Trieste (Italy), 9-11 January 1997.

13. Parallel algorithms for the calculation of electronic excitations
    G.-M. Rignanese, S. G. Louie, X. Blase, and A. C. Canning
    CECAM Workshop on Calculation of Electronic Excitations in Finite and Infinite Systems
    Lyon (France), 1-3 September 1999.

14. Quasiparticle band structure of C_2H_4 adsorbed on the Si(001)-2×1 surface within the approximation
    G.-M. Rignanese, S. G. Louie, and X. Blasé
    International Conference on Density Functional Theory and its Applications to Materials
    University of Antwerp, Antwerp (Belgium), 8-10 June 2000.

15. First-principles study of structural, dynamical, and dielectric properties of zirconium silicates
    G.-M. Rignanese, X. Gonze, and A. Pasquarello
    10th International Workshop on Computational Condensed-Matter Physics
    International Center for Theoretical Physics, Trieste (Italy), 11-13 January 2001.

16. First-principles study of structural and electronic properties of NiC phases
    M. Verstraete, G.-M. Rignanese, and J.-C. Charlier
    10th International Workshop on Computational Condensed-Matter Physics
    International Center for Theoretical Physics, Trieste (Italy), 11-13 January 2001.

17. The self-assembly and the hydrogen bond in biological and bio-inorganic systems
    X. Rocquefelte, G.-M. Rignanese, J.-C. Charlier, X. Gonze, and M. Elstner
    1st International ABINIT Developer Workshop
    Université Catholique de Louvain, Louvain-la-Neuve (Belgium), 6-8 November 2002.

18. Dielectric constants of Zr silicate alloys: A first-principles study
    G.-M. Rignanese, F. Detraux, X. Gonze, A. Bongiorno, and A. Pasquarello

    – 1st International ABINIT Developer Workshop
      Université Catholique de Louvain, Louvain-la-Neuve (Belgium), 6-8 November 2002.

    – Fonctionnelle de la densité: de la molécule aux matériaux et systèmes complexes
      La Londe Les Maures (France), 4-6 February 2004.

20. Dielectric constants of Zr silicates: A first-principles study
    G.-M. Rignanese, F. Detraux, X. Gonze, A. Bongiorno, and A. Pasquarello
    11th International Workshop on Computational Condensed-Matter Physics
    International Center for Theoretical Physics, Trieste (Italy), 16-18 January 2003.

21. Ab initio study of the elastic properties of carbon nanotubes and graphitic systems

    – 11th International Workshop on Computational Condensed-Matter Physics
      International Center for Theoretical Physics, Trieste (Italy), 16-18 January 2003.

    – Ecole Thématique “Nanotubes: Science et Applications”,
      Aussois (France), 21 April-3 May 2003.

23. First-principles study of transition metal oxides and silicates as high-κ dielectrics
    G.-M. Rignanese, X. Gonze, and A. Pasquarello
    10th International Conference on the Applications of Density Functional Theory in Chemistry and Physics
    Vrije Universiteit Brussel, Brussels (Belgium), 7-12 September 2003.

24. Valence band offsets in Mo/SiO_2 structures
    A. De Souza Martins, Y.-M. Niquet, G.-M. Rignanese, and X. Gonze
    Progress in *Ab Initio* Computational Methods for Condensed Matter
    Gif-sur-Yvette (France), 8-10 January 2004.

25. First-principles investigation of high-κ dielectrics
    G.-M. Rignanese
    12th International Workshop on Computational Condensed-Matter Physics
    International Center for Theoretical Physics, Trieste (Italy), 13-15 January 2005.

26. Ab initio electronic, structural and vibrational properties of small diameter nanotubes
    G.-M. Rignanese, D. Connétable, J.-C. Charlier, and X. Blase
    12th International Workshop on Computational Condensed-Matter Physics
    International Center for Theoretical Physics, Trieste (Italy), 13-15 January 2005.

27. The ideal strength of silicon : an ab initio study
    S.M.-M. Dubois, G.-M. Rignanese, T. Pardoen, and J.-C. Charlier
    12th International Workshop on Computational Condensed-Matter Physics
    International Center for Theoretical Physics, Trieste (Italy), 13-15 January 2005.

28. Ab initio transport properties of nanostructures
    C. Morari, S. Melinte, G.-M. Rignanese, J.-C. Charlier, and X. Gonze
    12th International Workshop on Computational Condensed-Matter Physics
    International Center for Theoretical Physics, Trieste (Italy), 13-15 January 2005.

29. Quasiparticle calculations of high-k materials band offsets with silicon
    R. Shaltaf and G.-M. Rignanese,
    356th Wilhelm and Else Heraeus Seminar: "40 Years of the GW Approximation"
    Physikzentrum, Bad Honnef (Germany), 12-15 September 2005

30. The transpost properties of alcanes and π-bonded molecules: the issue of cooperativity
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39. Transparent Conducting Oxides (TCO): tin oxides as a case study
A. Miglio, M. Stankovski, G. Geadah-Antonius, M. Giantomassi, G.-M. Rignanese, and X. Gonze

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41. GW defect formation energies of hydrogen containing silica
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50. Quasiparticle gap and optical absorption spectra of crystalline and amorphous silica including excitonic effects
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