Oral communications at professional meetings

1. Aluminium / Polystyrene Interface: Calculations on model systems and comparison to Secondary Ion Mass Spectroscopy (SIMS) data
   Y. Travaly, P. Bertrand, X. Gonze, and G.-M. Rignanese
   International Conference on Adhesion Science & Technology (ICAST ’95)
   Amsterdam (The Netherlands), 15-20 October 1995.

2. Parallelisation of algorithms for ab initio computation of material properties
   G.-M. Rignanese, J.-M. Beuken, J.-P. Michenaud, and X. Gonze
   7th European Convex Users' Conference (ECUC ’95)

3. Ab initio study of SiO$_2$ (α-quartz) surface
   G.-M. Rignanese, J.-P. Michenaud, X. Gonze, and Ph. Lambin
   1996 March meeting of the American Physical Society
   St Louis MO (USA), 18-22 March 1996.

4. The Aluminium/Poly (ethylene terephthalate) interface: A density functional theory study
   Y. Travaly, P. Bertrand, X. Gonze, and G.-M. Rignanese
   International Conference on Polymer-Solid Interfaces: from model to real systems (ICPSI-2)
   Namur (Belgium), 12-16 August 1996.

5. Aluminium/Polymers interfaces: calculations on model systems and comparison to experiments
   Y. Travaly, P. Bertrand, X. Gonze, and G.-M. Rignanese
   EURADH ’96
   Cambridge (UK), 3-6 September 1996.

6. 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
   – 1997 March meeting of the American Physical Society
     Kansas City MO (USA), 17-21 March 1997.
   – 16th General Conference of Condensed-Matter Division of the European Physical Society
   – 1st Topical Meeting on Heterostructures and Thin Films / Magnetism
     of the Interuniversity Attraction Pole on Reduced Dimensionality systems
     Namur (Belgium), 2 September 1997.

9. The Aluminium/Poly (ethylene terephthalate) interface: A density functional theory study
   Y. Travaly, P. Bertrand, X. Gonze, and G.-M. Rignanese
   1997 March meeting of the American Physical Society
   Kansas City MO (USA), 17-21 March 1997.

10. Core-level shifts in Si(001)-SiO$_2$ systems: The value of first-principle investigations
    (invited talk)
    A. Pasquarello, M. S. Hybertsen, G.-M. Rignanese, and R. Car
    NATO ASI Meeting on ‘Nanostructured Materials: Science and Technology’
    S. Petersburg (Russia), 11-21 August 1997.

11. Core-level Shifts at the nitrided Si(001)/SiO$_2$: Interface: a First-Principles Study
    (invited talk)
    G.-M. Rignanese, A. Pasquarello, J.-C. Charlier, X. Gonze, and R. Car
    CECAM Workshop on Simulation of Silicas
    Lyon (France), 15-17 September 1997.

12. Ab initio study of the (0001) α-Quartz surface
    (invited talk)
    CECAM Workshop on Simulation of Silicas
    Lyon (France), 15-17 September 1997.
   X. Gonze, G.-M. Rignanese, and J.-M. Beuken
   1998 March meeting of the American Physical Society.
   Los Angeles CA (USA), 16-20 March 1998.

14. Etude ab initio de la surface du SiO₂ et de son interface avec le Si
   G.-M. Rignanese
   4ème réunion du GDR ‘Liaison chimique dans le solide’

15. Etude ab initio de l’incorporation d’azote à l’interface Si(001)-SiO₂
   G.-M. Rignanese
   3ème réunion du GDR ‘Interface Métal/Oxydes’
   Saint-Hugues de Biviers (France), 16-18 November 1998.

16. GW calculations for spin-polarized systems
   G.-M. Rignanese, J.-L. Li, E. Chang, S. G. Louie, and X. Blase
   – 1999 March meeting of the American Physical Society
     Atlanta GO (USA), 20-26 March 1999.
   – Second Meeting of the EU Research and Training Network ‘Exciting’
     Louvain-la-Neuve (Belgium), 14-16 April 2003.

18. Quasiparticle band structure of C₆H₄ adsorbed on the Si(001)-2×1 surface within the GW approximation
   G.-M. Rignanese, S. G. Louie, and X. Blase
   – 2000 March meeting of the American Physical Society
     Minneapolis MN (USA), 20-24 March 2000.
   – CECAM Workshop on Excited States and Electronic Spectra
     Lyon (France), 20-22 July 2000.
   – Meeting of the work group on ‘Modelling’ of the COST Action 523
     ‘Nanostructured Materials’ of the European Union
     Brussels (Belgium), 3-4 November 2000.
   – First Meeting of the EU Research and Training Network ‘Exciting’
     Graz (Austria), 4-6 April 2002.

22. Quasiparticle Energy Bands of NiO in the approximation
   J.-L. Li, G.-M. Rignanese, and S. G. Louie
   2000 March meeting of the American Physical Society
   Minneapolis MN (USA), 20-24 March 2000.

23. First-Principle Calculation of Quasiparticle Excitations and Optical Adsorption in NiO
   J.-L. Li, G.-M. Rignanese, and S. G. Louie
   2001 March meeting of the American Physical Society
   Seattle WA (USA), 12-16 March 2001.

24. First-Principles study of structural, electronic, dynamical, and dielectric properties of zirconium silicates
   G.-M. Rignanese, X. Gonze, and A. Pasquarello
   2001 March meeting of the American Physical Society
   Seattle WA (USA), 12-16 March 2001.
25. Interpretation of N 1s core-level shifts at nitrided Si(001) surfaces and Si(001)-SiO₂ interfaces: A first-principles study
G.-M. Rignanese and A. Pasquarello
International Workshop on Device Technology
Porto Alegre (Brazil), 3-5 September 2001.

26. Dielectric constants of Zr silicate alloys: A first-principles study
G.-M. Rignanese, F. Detraux, X. Gonze, A. Bongiorno, and A. Pasquarello
2002 March meeting of the American Physical Society
Indianapolis IN (USA), 18-22 March 2002.

27. La liaison hydrogène dans des systèmes biologiques: comparaison de plusieurs codes
X. Rocquefelte, G.-M. Rignanese, J.-C. Charlier, X. Gonze, P. Koenig, and M. Elstner
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
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
G.-M. Rignanese, J.-C. Charlier, and X. Gonze
CECAM Workshop on Understanding the similarities of SiO₂, H₂O and other systems with tetrahedral local order
Lyon (France), 22-24 July 2002.

31. Calculating GW corrections with ABINIT
V. Olevano, R. Godby, L. Reining, G. Onida, M. Torrent, and G.-M. Rignanese
1st International ABINIT Developer Workshop
Louvain-la-Neuve (Belgium), 6-8 November 2002.

32. First-principles study of vibrational and dielectric properties of C₃N₄ polymorphs
G.-M. Rignanese, J.-C. Charlier, and X. Gonze
2003 March meeting of the American Physical Society
Austin TX (USA), 3-7 March 2003.

33. Transition metal oxides and silicates as high-κ dielectrics: a first-principles investigation
G.-M. Rignanese, X. Gonze, and A. Pasquarello
2003 March meeting of the American Physical Society
Austin TX (USA), 3-7 March 2003.

34. First-principles investigation of hydration and dehydration mechanisms of SiO₂ surface
G.-M. Rignanese, J.-C. Charlier, and X. Gonze
81st International Bunsen Discussion Meeting “Interfacial Water in Chemistry and Biology”
Velen (Germany), 19-23 September 2003.

35. Transition metal oxides and silicates as high-κ dielectrics: a first-principles investigation
G.-M. Rignanese, X. Gonze, and A. Pasquarello
International Congress on Materials Science and Nanotechnologies (European Academy of Science)
Brussels (Belgium), 22-24 October 2003.
36. Dielectric properties of crystalline and amorphous transition metal oxides and silicates  
   (invited talk)  
   G.-M. Rignanese  
   2004 March meeting of the American Physical Society  
   Montréal (Canada), 22-26 March 2004.  

37. First-principles study of crystalline and amorphous transition metal oxides and silicates  
   (invited talk)  
   G.-M. Rignanese  
   CECAM Workshop on Atomic processes at semiconductor-oxide interfaces in microelectronic devices  
   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.  

42. Electronic and dielectric properties of group IVB transition metal oxides  
   (invited talk)  
   G.-M. Rignanese  
   International Symposium on Structure-Property Relationships in Solid State Materials  

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  
   11$^{th}$ 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  
   212$^{th}$ 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  
   13$^{th}$ Nanoquanta/ETSF Conference: Theoretical Spectroscopy and Quantum Transport  

47. Electronic Transport in zig-zag Graphene Nanoribbons  
   S. M.-M. Dubois, G.-M. Rignanese, and J.-C. Charlier  
   13$^{th}$ Nanoquanta/ETSF Conference: Theoretical Spectroscopy and Quantum Transport  
48. Band offsets from Many-Body Perturbation Theory

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

CECAM Workshop “Which Electronic Structure Method for the Study of Defects?”
Lausanne (Switzerland), 8-10 June 2009.


G.-M. Rignanese

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. Stankovski, A. Miglio, G. Geadah-Antonius, M. Giantomassi, G.-M. Rignanese, and X. Gonze

14th ETSF Conference: Theoretical Spectroscopy and Quantum Transport
Evora (Portugal), 14-19 September 2009.

52. Quantum Transport in Graphene Nanoribbons

S. M.-M. Dubois, G.-M. Rignanese, and J.-C. Charlier

14th ETSF Conference: Theoretical Spectroscopy and Quantum Transport
Evora (Portugal), 14-19 September 2009.

53. Calcul des décalages de bandes aux interfaces: de la DFT à l’approximation GW

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

T. Rangel, A. Ferretti, P.E. Trevisanutto, V. Olevano, and G.-M. Rignanese

15th ETSF Conference: Theoretical Spectroscopy and Quantum Transport
Berlin (Germany), 12-15 October 2010.

56. What is the $G_0W_0$ band-gap of ZnO


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

M. Stankovski, G. Antonius, A. Miglio, D. Waroquiers, M. Côté, X. Gonze, and G.-M. Rignanese

16th ETSF Conference: Theoretical Spectroscopy and Quantum Transport
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: Theoretical Spectroscopy and Quantum Transport
Torino (Italy), 27-30 September 2011.

59. The ABINIT software project

G.-M. Rignanese

2011 One-day Workshop on Optimization in Materials Computing
Beijing (China), 16 November 2011.