

Oral communications at professional meetings

1. Aluminium / Polystyrene Interface:
Calculations on model systems and comparison to Secondary Ion Mass Spectroscopy (SIMS) data
Y. Travalay, 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)
Brussels (Belgium), 25-27 October 1995.
3. Ab initio study of SiO₂ (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.
Abstract in Bull. Am. Phys. Soc. **41**, 259 (1996)
4. The Aluminium/Poly (ethylene terephthalate) interface: A density functional theory study
Y. Travalay, 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. Travalay, P. Bertrand, X. Gonze, and G.-M. Rignanese
EURADH '96
Cambridge (UK), 3-6 September 1996.
6. Nitrogen Incorporation at the Si(001)/SiO₂ 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
Leuven (Belgium), 25-28 August 1997.
 - 1st Topical Meeting on Heterostructures and Thin Films / Magnetism
of the Interuniversity Attraction Pole on Reduced Dimensionality systems
Namur (Belgium), 2 September 1997.Abstract in Bull. Am. Phys. Soc. **42**, 378 (1997).
9. The Aluminium/Poly (ethylene terephthalate) interface: A density functional theory study
Y. Travalay, P. Bertrand, X. Gonze, and G.-M. Rignanese
1997 March meeting of the American Physical Society
Kansas City MO (USA), 17-21 March 1997.
Abstract in Bull. Am. Phys. Soc. **42**, 635 (1997).
10. Core-level shifts in Si(001)-SiO₂ 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. N 1s Core-level Shifts at the nitrated Si(001)/SiO₂ 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)
G.-M. Rignanese, J.-P. Michenaud, X. Gonze, X. Blase, J.-C. Charlier, A. De Vita, and R. Car
CECAM Workshop on Simulation of Silicas
Lyon (France), 15-17 September 1997.

13. A potential-based conjugate-gradient algorithm for electronic-structure and total-energy calculations
 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.
 Abstract in Bull. Am. Phys. Soc. **43**, 66 (1998).
14. Etude ab initio de la surface du SiO₂ et de son interface avec le Si (invited talk)
 G.-M. Rignanese
 4^{ème} réunion du GDR ‘Liaison chimique dans le solide’
 Paris (France), 2-3 July 1998.
15. Etude ab initio de l'incorporation d'azote à l'interface Si(001)-SiO₂ (invited talk)
 G.-M. Rignanese
 3^{ème} 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 GA (USA), 20-26 March 1999.
 – Second Meeting of the EU Research and Training Network ‘Exciting’
 Louvain-la-Neuve (Belgium), 14-16 April 2003.
 Abstract in Bull. Am. Phys. Soc. **44**, 1667 (1999).
18. Quasiparticle band structure of C₂H₄ 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 (invited talk)
 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.
 Abstract in Bull. Am. Phys. Soc. **45**, 865 (2000).
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.
 Abstract in Bull. Am. Phys. Soc. **45**, 922 (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.
 Abstract in Bull. Am. Phys. Soc. **46**, 132 (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.
 Abstract in Bull. Am. Phys. Soc. **46**, 1004 (2001).

25. Interpretation of N 1s core-level shifts at nitrated Si(001) surfaces and Si(001)-SiO₂ interfaces: A first-principles study (invited talk)
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.
 Abstract in Bull. Am. Phys. Soc. **47**, 968 (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 (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
 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.
 Abstract in Bull. Am. Phys. Soc. **48**, 302 (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.
 Abstract in Bull. Am. Phys. Soc. **48**, 964 (2003).
34. First-principles investigation of hydration and dehydration mechanisms of SiO₂ surface (invited talk)
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 (invited talk)
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.
 Abstract in Bull. Am. Phys. Soc. 49, 89 (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
 Bordeaux (France), 27-30 June 2006.
43. First-Principles Calculations of Band Offsets of SiO₂ and ZrSiO₄ 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: Theoretical Spectroscopy and Quantum Transport
 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: Theoretical Spectroscopy and Quantum Transport
 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 (invited talk)
G.-M. Rignanese
 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 (invited talk)
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-Antonijs, 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 (invited talk)
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 (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. Trevisanuto, 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 (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: 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 (invited talk)
G.-M. Rignanese
 2011 One-day Workshop on Optimization in Materials Computing
 Beijing (China), 16 November 2011.