

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 **52**, 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)/SiO₂ 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 NH₃ 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 nitrated Si(001) surfaces and Si(001)-SiO₂ 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 C₂H₄ 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 NH₃ saturated Si(100)-2×1 surface: a first-principles study
G.-M. Rignanese and A. Pasquarello
Surf. Sci. **490**, L614-L618 (2001)
13. Electronic structure of carbon nanocones
J.-C. Charlier and G.-M. Rignanese
Phys. Rev. Lett. **86**, 5970-5973 (2001)
14. GW study of the metal-insulator transition of bcc hydrogen
J.-L. Li, G.-M. Rignanese, E. K. Chang, X. Blase, and S. G. Louie
Phys. Rev. B **66**, 035102:1-5 (2002)

15. 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)
16. 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)
17. First-principles study of vibrational and dielectric properties of C₃N₄ polymorphs
G.-M. Rignanese, J.-C. Charlier, and X. Gonze
Phys. Rev. B **66**, 205416:1-6 (2002)
18. Superconductivity in doped *sp*³ semiconductors: the case of clathrates
D. Connétable, V. Timoshevskii, B. Masenelli, J. Beille, J. Marcus, B. Barbara, A.M. Saitta, G.-M. Rignanese, P. Mélinon, S. Yamanaka, and X. Blase
Phys. Rev. Lett. **91**, 247001:1-4 (2003)
19. First-principles molecular-dynamics investigation of the hydration mechanisms of the (0001) α -quartz surface
G.-M. Rignanese, J.-C. Charlier, and X. Gonze
Phys. Chem. Chem. Phys. **6**, 1920-1925 (2004)
20. How to Identify Haeckelite Structures: A Theoretical Study of Their Electronic and Vibrational Properties
X. Rocquefelte, G.-M. Rignanese, V. Meunier, H. Terrones, M. Terrones, and J.-C. Charlier
Nano Lett. **4**, 805-810 (2004)
21. 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)
22. Titanium oxides and silicates as high- κ dielectrics: A first-principles investigation
G.-M. Rignanese, X. Rocquefelte, X. Gonze, and A. Pasquarello,
Int. J. Quantum Chem. **101**, 793-801 (2005)
23. 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)
24. Dielectric properties of crystalline and amorphous transition metal oxides and silicates as potential high- κ candidates: the contribution of density-functional theory
G.-M. Rignanese
J. Phys.: Condens. Matter **17**, R357-R379 (2005)
25. Modelling of dielectric constants of amorphous Zr silicates
G.-M. Rignanese and A. Pasquarello,
J. Phys.: Condens. Matter **17**, S2089-S2098 (2005)
26. First-principle studies of the lattice dynamics of crystals, and related properties
X. Gonze, G.-M. Rignanese, R. Caracas
Z. Kristallogr. **220**, 458-472 (2005)
27. 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)
28. Quasiparticle energy bands of NiO in the GW approximation
J.-L. Li, G.-M. Rignanese, and S. G. Louie
Phys. Rev. B **71**, 193102:1-4 (2005)

29. Ideal strength of silicon: An *ab initio* study
S. M.-M. Dubois, G.-M. Rignanese, T. Pardoen, and J.-C. Charlier,
Phys. Rev. B **74**, 235203:1-7 (2006)
30. Electronic properties of 1-4, dicyanobenzene and 1-4, phenylene diisocyanide molecules contacted between Pt and Pd electrodes: First-principles study
C. Morari, G.-M. Rignanese, and S. Melinte
Phys. Rev. B **76**, 115428:1-6 (2007)
31. Hybrid exchange-correlation functional for accurate prediction of the electronic and structural properties of ferroelectric oxides
D. I. Bilc, R. Orlando, R. Shaltaf, G.-M. Rignanese, J. Iniguez, and Ph. Ghosez
Phys. Rev. B **77**, 165107:1-13 (2008)
32. Band Offsets at the Si/SiO₂ 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)
33. Hyptothetical three-dimensional all-sp² carbon phase
G.-M. Rignanese and J.-C. Charlier
Phys. Rev. B **78**, 125415:1-5 (2008)
34. Electronic properties of zircon and hafnon from many-body perturbation theory
R. Shaltaf, T. Rangel, M. Grüning, X. Gonze, G.-M. Rignanese, and D.R. Hamann
Phys. Rev. B **79**, 195101:1-6 (2009)
35. ABINIT: First-principles approach to material and nanosystem properties
X. Gonze, B. Amadon, P.-M. Anglade, J.-M. Beuken, F. Bottin, P. Boulanger, F. Bruneval, D. Caliste, R. Caracas, M. Côté, T. Deutsch, L. Genovese, Ph. Ghosez, M. Giantomassi, S. Goedecker, D.R. Hamannm, P. Hermet, F. Jollet, G. Jomard, S. Leroux, M. Mancini, S. Mazevet, M.J.T. Oliveira, G. Onida, Y. Pouillon, T. Rangel, G.-M. Rignanese, D. Sangalli, R. Shaltaf, M. Torrent, M.J. Verstraete, G. Zerah, J.W. Zwanziger
Comput. Phys. Commun. **180**, 2582-2615 (2009)
36. Electronic Transport Properties of 1,1'-Ferrocene Dicarboxylic Acid Linked to Al(111) Electrodes
C. Morari, I. Rungger, A. R. Rocha, S. Sanvito, S. Melinte, and G.-M. Rignanese
ACS Nano **3**, 4137-4143 (2009)
37. Quasiparticle calculations of the electronic properties of ZrO₂ and HfO₂ polymorphs and their interface with Si
M. Grüning, R. Shaltaf, and G.-M. Rignanese
Phys. Rev. B **81**, 035330:1-7 (2010)
38. First-principles modeling of intrinsic and extrinsic defects in γ -Al₂O₃
K. Sankaran, G. Pourtois, R. Degraeve, M. B. Zahid, G.-M. Rignanese, and J. Van Houdt
Appl. Phys. Lett. **97**, 212906:1-3 (2010)
39. Electronic properties of interfaces and defects from many-body perturbation theory: Recent developments and applications
M. Giantomassi, M. Stankovski, R. Shaltaf, M. Grüning, F. Bruneval, P. Rinke, and G.-M. Rignanese
Phys. Status Solidi B **248**, 275-289 (2011)
40. Convergence of quasiparticle band structures of Si and Ge nanowires in the GW approximation and the validity of scissor shifts
H. Peelaers, B. Partoens, M. Giantomassi, T. Rangel, E. Goossens, G.-M. Rignanese, X. Gonze, and F.M. Peeters
Phys. Rev. B **83**, 045306:1-6 (2011)
41. Transport properties of molecular junctions from many-body perturbation theory
T. Rangel, A. Ferretti, P.E. Trevisanutto, V. Olevano, and G.-M. Rignanese,
Phys. Rev. B **84**, 045426:1-5 (2011)
42. G⁰W⁰ band gap of ZnO: Effects of plasmon-pole models
M. Stankovski, G. Antonius, D. Waroquiers, A. Miglio, H. Dixit, K. Sankaran, M. Giantomassi,
X. Gonze, M. Côté, and G.-M. Rignanese,
Phys. Rev. B **84**, 241201(R):1-5 (2011)

43. Electronic Properties of Hybrid Zinc Oxide–Oligothiophene Nanostructures
C. Caddeo, G. Mallocci, G.-M. Rignanese, L. Colombo, and A. Mattoni,
J. Phys. Chem. C **116**, 8174–8180 (2012)
44. Band structure of gold from many-body perturbation theory
T. Rangel, D. Kecik, P.E. Trevisanutto, G.-M. Rignanese, H. Van Swygenhoven, and V. Olevano
Phys. Rev. B **86**, 125125:1-9 (2012)
45. Effects of plasmon pole models on the G^0W^0 electronic structure of various oxides
A. Miglio, D. Waroquiers, G. Antonius, M. Giantomassi, M. Stankovski, M. Côté, X. Gonze, and G.-M. Rignanese
Eur. Phys. J. B **85**, 322 (2012)

B. Book chapters

1. Core-level shifts in Si(001)-SiO₂ systems: The value of first-principle investigations
A. Pasquarello, M. S. Hybertsen, G.-M. Rignanese, and R. Car
Fundamental Aspects of Ultrathin Dielectrics on Si-based Devices
edited by E. Garfunkel, E. Gusev and A. Vul (Kluwer, Dordrecht, 1998), pp 89-102
2. The fundamental state of poly(ethylene terephthalate) and its interaction with evaporated aluminum
Y. Travaly, G.-M. Rignanese, X. Gonze, and P. Bertrand
Metallized Plastics 7: Fundamental and Applied Aspects
edited by K. L. Mittal (VSP, Zeist, 2001), pp. 247-264
3. Ab-initio calculations of the structural, electronic and dynamical properties of high-k dielectrics
G.-M. Rignanese, X. Gonze, and A. Pasquarello,
High-k dielectrics
edited by M. Houssa (Institute of Physics Publishing, Bristol, 2004), pp 431-466
4. IVb Transition Metal Oxides and Silicates: An Ab Initio Study
G.-M. Rignanese
Materials Fundamentals of Gate Dielectrics
edited by A. A. Demkov and A. Navrotsky (Springer, Dordrecht, 2005), pp 249-290
5. Electronic properties of interfaces and defects from many-body perturbation theory: Recent developments and applications
M. Giantomassi, M. Stankovski, R. Shaltaf, M. Grüning, F. Bruneval, P. Rinke, and G.-M. Rignanese
Advanced Calculations for Defects in Materials
edited by A. Alkauskas, P. Deák, J. Neugebauer, A. Pasquarello, and C.G. Van de Walle
(Wiley-VCH, Weinheim, 2011), pp 33-60.

C. Conference papers

1. Parallelisation of algorithms for ab initio computation of material properties
G.-M. Rignanese, J.-M. Beuken, J.-P. Michenaud, and X. Gonze
Proceedings of the 7th European Convex Users' Conference (ECUC '95)
2. The Aluminium/Poly (ethylene terephthalate) interface: A density functional theory study
Y. Travaly, P. Bertrand, X. Gonze, and G.-M. Rignanese
Proceedings of the International Conference on Polymer-Solid Interfaces: from Model to Real Systems (PUN, Namur, 1998), pp. 453-465
3. Aluminium/Polymers interfaces: calculations on model systems and comparison to experiments
Y. Travaly, P. Bertrand, X. Gonze, and G.-M. Rignanese
Proceedings of EURADH '96 (The Institute of Materials, Cambridge, 1996), pp. 71-75
4. Interpretation of N 1s core-level shifts at nitrated Si(001) surfaces and Si(001)-SiO₂ interfaces: A first-principles study
G.-M. Rignanese and A. Pasquarello
Alternatives to SiO₂ as Gate Dielectrics for Future Si-Based Microelectronics
edited by J. Morais and I.J.R. Baumvol (MRS Workshop Series, 2001), pp 24:1-10
5. First-Principles Study of Dynamical and Dielectric Properties of Orthorhombic Phases of Group IVb Transition Metal Oxides
G.-M. Rignanese

Electrochem. Soc. Trans. **11**(4), 47-58 (2007)

6. First-Principles Investigation of High-k Dielectrics for Nonvolatile Memories
G. Pourtois, K. Sankaran, I. Radu, R. Degraeve, M. B. Zahid, S. Van Elshocht, C. Adelman, S. De Gendt, M. M. Heyns, D. J. Wouters, J. A. Kittl, M. Jurczak, G.-M. Rignanese, and J. Van Houdt
Electrochem. Soc. Trans. **33**(3), 393-407 (2010)
7. Modeling Of Copper Diffusion In Amorphous Aluminum Oxide in CBRAM Stack
K. Sankaran, L. Goux, S. Clima, M. Mees, J. Kittl, M. Jurczak, L. Altimime, G.-M. Rignanese, and G. Pourtois,
Electrochem. Soc. Trans. **45**(3), 317-330 (2012)
8. Field-driven ultrafast sub-ns programming in WAl₂O₃/Ti/CuTe-based 1T1R CBRAM system
L. Goux, K. Sankaran, G. Kar, N. Jossart, K. Opsomer, R. Degraeve, G. Pourtois, G.-M. Rignanese, C. Detavernier, S. Clima, Y.-Y. Chen, A. Fantini, B. Govoreanu, D.J. Wouters, M. Jurczak, L. Altimime, and J.A. Kittl,
2012 Symposium on VLSI Technology Digest of Technical Papers, 69-70 (2012)

D. Popularization articles

1. Le Prix Nobel de Chimie: Les quasi-cristaux
G.-M. Rignanese
Rev. Quest. Sci. **182**, 117-126 (2012)