Dr. Fabien Bruneval

Age:	35
Born:	May 1st 1979
Marital status:	married, 2 children
Citizenship:	French
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Current position: (since Dec. 2007)

Dec. 2007 –	Permanent Researcher at CEA (Atomic Energy Commission) Service de Recherches de Métallurgie Physique CEA Saclay, France
Aug. 2014 – July 2015:	Visiting scholar at UC Berkeley (USA) in the group of Prof. J.B. Neaton

Former positions:

Jan. 2006 – Nov. 2007:	Post-doctoral researcher at **ETH Zurich**, Department of Chemistry and Applied Biosciences, Switzerland supervisor: Prof. Michele Parrinello
Oct. 2005 – Dec. 2005:	Post-doctoral researcher at **Ecole Polytechnique**, Laboratoire des Solides Irradiés, France supervisors: Dr. Lucia Reining and Dr. Nathalie Vast

Education:

June 2014 (scheduled):	Professional qualification “Habilitation à diriger des Recherches” “Electronic structure of point defects in semiconductors” at Ecole doctorale de **l’université C. Bernard Lyon I**, France.
2002 – 2005:	PhD in Physics at **Ecole Polytechnique**, France “Exchange and correlation in solids, from silicon to cuprous oxyde” supervisors: Dr. Nathalie Vast and Dr. Lucia Reining

2001 – 2002:	Master of Science in Material Science at **University Pierre et Marie Curie - Paris VI**
1999 – 2002:	Engineering degree at **Ecole Centrale Paris**, France specialization in Applied Physics

Scientific publication highlights:

Number of peer-reviewed articles:	33
Book chapters:	2
H-index:	16

Most cited articles (> 50 citations in ISI-database as of October 2014):

1. *ABINIT: First-principles approach to material and nanosystem properties*, X. Gonze *et al.*, Comput. Phys. Commun. **180**, 2582 (2009).

   615 citations

2. *A brief introduction to the ABINIT software package*, X. Gonze *et al.,* Z. Kristallogr. **220**, 558 (2005).
   592 citations

3. *Effect of self-consistency on quasiparticles in solids*, F. Bruneval, N. Vast, and L. Reining, Phys. Rev. B **74**, 045102 (2006).

   110 citations

4. *Understanding correlations in vanadium dioxide from first principles*, M. Gatti, F. Bruneval, V. Olevano, and L. Reining, Phys. Rev. Lett. **99**, 266402 (2007).

   84 citations

5. *Accurate GW self-energies in a plane-wave basis using only a few empty states: Towards large systems,* F. Bruneval and X. Gonze, Phys. Rev. B **78**, 085125 (2008).

   68 citations

6. *Many-body perturbation theory using the density-functional concept: Beyond the GW approximation*, F. Bruneval *et al.*, Phys. Rev. Lett. **94**, 186402 (2006).

   67 citations

7. *Exchange and correlation effects in electronic excitations of Cu2O*, F. Bruneval *et al.*, Phys. Rev. Lett. **97**, 267601 (2006).

   54 citations

Invited conference communications:

June 2015 *GW for chemists*
in ISTPC 2015, summer school in Aussois (France).

July 2014 *Recent advances in the electronic structure calculations of charged defects*, in ICMR workshop "Charged systems and solid/liquid interfaces from first principles", Santa Barbara (USA)

March 2013 *Hybrid functionals in Abinit à la GW*,
in Abinit 6th developers' workshop, Dinard, (France)

June 2011 *The GW approximation when the number of particles changes for real*, in CECAM workshop "Challenges and Solutions in GW Calculations for Complex Systems", Lausanne (Switzerland)

April 2011 *The RPA total energy in Abinit*,
in Abinit 5th developers' workshop, Han-sur-Lesse, (Belgium)

Nov. 2010 *The GW approximationin less than 60 minutes,*
in "First Yarmouk School for Computational Condensed Matter and Nano Systems", Irbid (Jordan)

Sept. 2010 *GW approximation for electron number changes: application to point defects,*
in Psik conference 2010, Berlin (Germany)

Sept. 2009 *Approche GW pour les défauts chargés dans les isolants*
in final workshop of the ANR project LN3M, Lyon (France)

May 2009 *Introduction to the GW approximation*
in CECAM tutorial "Theoretical Spectroscopy Lectures: theory and codes", Zurich (Switzerland)

Dec. 2007 *Introduction to the GW approximation*
in CECAM tutorial "Theoretical Spectroscopy Lectures: theory and codes", Lyon (France)

Jan. 2007 *Self-consistent GW electronic structure of solids*
in "13 th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods", Trieste (Italy)

Dec. 2006 *Introduction to the GW approximation*
in CECAM tutorial "Electronic excitations and spectroscopies : Theory and Codes", Lyon (France)

Sept. 2005 *Electronic Structure of Cu2O within self-consistent GW*
in "The 2005 Nanoquanta Workshop", Bad Honnef (Germany)

Teaching:

- Tutorial classes "Quantum and statistical physics", Ecole Centrale Paris (France), 3rd year of university
  2012: 55 hours
  2013: 55 hours
  2014: 55 hours

- Tutorial classes in “Solid-State Physics”, Ecole Centrale Paris (France), 4th year of university
  2012: 18 hours

Jury:

- External reviewer for the PhD thesis of David Waroquiers, Université Catholique de Louvain-la-Neuve (Jan. 2013)

Conference organization:

- Workshop organizer at Centro Stefano Frascini “Nothing is perfect – the quantum mechanics of defects”, April 26-29 2015, Ascona (Switzerland).
- International organizing committee member of the “5th ABINIT International developer workshop”, April 11-14 2011, Han-sur-Lesse (Belgium)
- Local organizer of the “Nanoquanto Young Researchers' Meeting”, May 6-8 2004, Palaiseau (France)

Grants/Fundings:

- 2014-2015: **Enhanced Eurotalent program** laureate from CEA and Marie Curie Actions of FP7 (funding for a sabbatical leave)
- 2014-2015: **France-Berkeley Fund** laureate (funding for a sabbatical leave)
- 2009-2013: principal investigator for project “Materials for energy” granted by **GENCI** (high performance computational resources)
- 2011-2013: partner for MAD-FIZ project “Doping of ZnO nanowires” funded by **Agence Nationale de la Recherche** (funding for 2 years post-doctoral position)
- 2009-2011: principal investigator for project “p-type doping in ZnO” funded by **Advanced Material Program of CEA** (funding for 2 years post-doctoral position)

Mentoring:

- Post-docs:
  - Guido Petretto (2012-2014), “p-type doping in ZnO thick nanowires”
  - Ying Cui (2009-2011), “Doping capabilities of ZnO, a photovoltaic material”

- PhD students:
  - Abdullah Shukri (2012-), “Ab initio calculation of the electronic stopping power in materials”
  - Samuel E. Taylor (2010-2011), “Charged defects in supercells”

- Internship students:
  - 2012: Arnaud Bourasseau, Orsay University (France)
  - 2011: Hichem Ben Hamed, Tunis University (Tunisia)

Other activities in the scientific community:

- Member of the advisory board of the ab initio software **Abinit**
- Member of the committee for allocation of French high-performance computing resources (**GENCI** CT 9)
- Member of the board of the French research networks **GdR-DFT++** and then **GdR-coDFT**
- Reviewer for journals: *Physical Review B*, *Physical Review Letters*, *Journal of Physics: Condensed Matter*, *New Journal of Physics, Physica Status Solidi (b*), *Physica Status Solidi (c*), *Journal of Chemical Physics, Journal of Chemical Theory and Computation, Reports on Progress in Physics*, *European Physical Journal B*, *Nanotechnology*
- External reviewer for funding agencies: *National Science Foundation* (USA)*, Agence Nationale de la Recherche* (France)*, Swiss National Science Foundation* (Switzerland)*, Platform of Advanced Scientific Computing* (Switzerland), *PRACE Prioritization Panel* (EU)

Comprehensive publication list:

Book chapters:

1. *Quasiparticle self-consistent GW method for the spectral properties of complex materials*, F. Bruneval and M. Gatti, chapter in volume “First Principle Approaches to Spectroscopic Properties of Complex Materials”, Eds. C. Di Valentin, S. Botti, and M. Cococcioni, Springer series “Current topic in Quantum Chemistry” Vol. **347**, pp. 99-135 (2014).
2. *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, chapter in volume “Advanced Calculations for Defects in Materials”, Eds. A. Alkauskas, P. Deák, J. Neugebauer, A. Pasquarello, and C.G. Van de Walle, Wiley-VCH, pp 33-60 (2011).

Peer-reviewed articles:

1. *Comprehensive Ab Initio Study of Doping in Bulk ZnO with Group-V Elements,*
   G. Petretto and F. Bruneval,
   Phys. Rev. Applied **1**, 024005 (2014).
2. *Screened Coulomb interaction calculations: cRPA implementation and applications to dynamical screening and self-consistency in uranium dioxide and cerium,*
   B. Amadon, Th. Applencourt, and F. Bruneval,
   Phys. Rev. B **89**, 125110 (2014).
3. *Consistent treatment of charged systems within periodic boundary conditions: The projector augmented-wave and pseudopotential methods revisited*,
   F. Bruneval, J.P. Crocombette, X. Gonze, B. Dorado, M. Torrent, and F. Jollet,
   Phys. Rev. B **89**, 045116 (2014).
4. *Point defect modeling in materials: Coupling ab initio and elasticity approaches*,
   C. Varvenne, F. Bruneval, M.C. Marinica, and E. Clouet,
   Phys. Rev. B **88**, 134102 (2013).
5. *Benchmarking the Starting Points of the GW Approximation for Molecules*,
   F. Bruneval and M. A. L. Marques,
   J. Chem. Theory Comput. **9**, 324 (2013).
6. *Ab initio formation volume of charged defects*,
   F. Bruneval and J.-P. Crocombette,
   Phys. Rev. B **86**, 140103(R) (2012).
7. *Formation and migration energy of native defects in silicon carbide from first principles: an overview*,
   G. Roma *et al.*,

Defect and Diffusion Forum **323-325**, 11 (2012).

8. *Range-Separated Approach to the RPA Correlation Applied to the van der Waals Bond and to Diffusion of Defects*,
   F. Bruneval,
   Phys. Rev. Lett. **108**, 256403 (2012).
9. *Ionization energy of atoms obtained from GW self-energy or from random phase approximation total energies*,
   F. Bruneval,
   J. Chem. Phys. **136**, 194107 (2012).
10. *Methodological aspects of the GW calculation of the carbon vacancy in 3C-SiC*,
    F. Bruneval,
    Nucl. Instrum. Meth. B **277**, 77 (2012).
11. *Direct observation of Al-doping-induced electronic states in the valence band and band gap of ZnO films*,
    M. Gabás *et al.*,
    Phys. Rev. B **84**, 153303 (2011).
12. *Understanding and correcting the spurious interactions in charged supercells,*
    S. E. Taylor and F. Bruneval,
    Phys. Rev. B **84**, 075155 (2011).
13. *Energetics and metastability of the silicon vacancy in cubic SiC*,
    F. Bruneval and G. Roma,
    Phys. Rev. B **83**, 144116 (2011).
14. *Electronic properties of interfaces and defects from many-body perturbation theory: Recent developments and applications*,
    M. Giantomassi *et al.*,
    Phys. Status Solidi B **248**, 275 (2011).
15. *p-type doping and codoping of ZnO based on nitrogen is ineffective: An ab initio clue*,
    Y. Cui and F. Bruneval,
    Appl. Phys. Lett. **97**, 042108 (2010).
16. *Effects of Electronic and Lattice Polarization on the Band Structure of Delafossite Transparent Conductive Oxides*,
    J. Vidal *et al.*, Phys. Rev. Lett. **104**, 136401 (2010).
17. *Dynamic structure factor and dielectric function of silicon for finite momentum transfer: Inelastic x-ray scattering experiments and ab initio calculations,*
    H. C. Weissker *et al.*,
    Phys. Rev. B **81**, 085104 (2010).
18. *ABINIT: First-principles approach to material and nanosystem properties*,
    X. Gonze *et al.*,
    Comput. Phys. Commun. **180**, 2582 (2009).

19. *GW Approximation of the Many-Body Problem and Changes in the Particle Number*, F. Bruneval, Phys. Rev. Lett. **103**, 176403 (2009).
20. *A Molecular Dynamics Study of the Early Stages of Calcium Carbonate Growth*, G.A. Tribello, F. Bruneval, C.C. Liew and M. Parrinello, J. Phys. Chem. B **113**, 11680 (2009).
21. *Accurate GW self-energies in a plane-wave basis using only a few empty states: Towards large systems,* F. Bruneval and X. Gonze, Phys. Rev. B **78**, 085125 (2008).
22. *New Lennard-Jones metastable phase,* H. Eshet, F. Bruneval, and M. Parrinello, J. Chem. Phys. **129**, 026101 (2008).
23. *Molecular dynamics study of the solvation of calcium carbonate in water*, F. Bruneval, D. Donadio, and M. Parrinello, J. Phys. Chem. B **111**, 12219 (2007).
24. *Understanding correlations in vanadium dioxide from first principles*, M. Gatti, F. Bruneval, V. Olevano, and L. Reining, Phys. Rev. Lett. **99**, 266402 (2007).
25. *Electronic excitations: Ab initio calculations of electronic spectra and application to zirconia ZrO_2, titania TiO_2 and cuprous oxide Cu_2O*, L. K. Dash *et al.*, Comput. Mater. Science **38**, 482 (2007).
26. *Exchange and correlation effects in electronic excitations of Cu_2O,* F. Bruneval *et al.*, Phys. Rev. Lett. **97**, 267601 (2006).
27. *Effect of self-consistency on quasiparticles in solids*, F. Bruneval, N. Vast, and L. Reining, Phys. Rev. B **74**, 045102 (2006).
28. *Beyond time-dependent exact exchange: The need for long-range correlation*, F. Bruneval, F. Sottile, V. Olevano, and L. Reining, J. Chem. Phys. **127**, 144113 (2006).
29. *Signatures of short-range many-body effects in the dielectric function of silicon for finite momentum transfer*, H.C. Weissker *et al.,* Phys. Rev. Lett. **97**, 237602 (2006).
30. *Many-body perturbation theory using the density-functional concept: Beyond the GW approximation*, F. Bruneval *et al.*,

Phys. Rev. Lett. **94**, 186402 (2006).

31. *A brief introduction to the ABINIT software package*,
X. Gonze *et al.,*
Z. Kristallogr. **220**, 558 (2005).

32. *Comment on “Quantum confinement and electronic properties of silicon nanowires”,*
F. Bruneval, S. Botti, and L. Reining,
Phys. Rev. Lett. **94**, 219701 (2005).

33. *TDDFT from molecules to solids: The role of long-range interactions*,
F. Sottile *et al.,*
Int. J. Quant. Chem. **102**, 684 (2005).