lucia.reining@polytechnique.fr • **Lucia Reining** • (33) 1 69334553

Directrice de Recherche au CNRS (1st class)
Coordinator of the LSI Theoretical Spectroscopy group
Vice-president, European Theoretial Spectroscopy Facility (ETSF)
Head of the ETSF Palaiseau node
Born: 13.9.1961. Married, 3 children (1992, 1995, 1995)

Laboratoire des Solides Irradiés
École Polytechnique
91128 Palaiseau
France

Education

- 1991, PhD thesis (Dottorato di Ricerca), Rome, Italy (Adv. R. Del Sole)
- 1985, Diploma thesis (Diplomarbeit), RWTH Aachen, Germany (Adv. I. Egry)
- 1980 - 1985, University RWTH Aachen, Physics

Positions

- 2009 - , 1st class Senior Reserchер (Directrice de Recherche) at the Centre National de la Recherche Scientifique (CNRS)
- 2006 - , Coordinator, Theoretical Spectroscopy group (permanent members: 7) of the Laboratoire des Solides Irradiés (LSI)
- 2002 - 2008, CNRS Senior Researcher (Directrice de Recherche)
- 2000 - 2006, Head, LSI Theory group (permanent members: 7)
- 1992 - 2002, CNRS Chargée de Recherche
- 1991-1992, Scientist, Marie Curie Post-Doc fellowship of the European Community, Centre Européen de Calcul Atomique et Moléculaire
- 1986 - 1987, Visiting Scientist, University "Tor Vergata", Rome, Italy

Main professional activities

European:

- 2008 - today, Vice-president "for Users and Technology" of the European Theoretical Spectroscopy Facility
  (ETSF, `www.etsf.eu`)
- 2008 - today, Deputy Coordinator of the European FP7 e-Infrastructure ETSF-I3
- 2008 - today, Member of the PsiK Scientific Advisory Committee
- 2007/2008, President *ad interim* of the ETSF
- 2004 - 2008, Deputy Coordinator of the European FP6 Network of Excellence NANOQUANTA (Nanoscale Quantum Simulations for Nanostructures and Advanced Materials)
- 2002 - 2006, Responsible of the Marie Curie Training site "LSI-Electronic structure"
- 2000 - 2004, Local Coordinator of the European FP5 RTN network NANOPHASE (Nanoscale photon absorption and spectroscopy with electrons)
- 1993 - 1995, Local Coordinator of the European FP3 network EPSI (Electronic Properties of Semiconductors and Insulators: Computing the Behaviour of Complex Systems)

Other not French:

- 2011 - today, Member of the scientific advisory board at the Max Planck Institute of Microstructure Physics in Halle
- 2007 - today, Member and vice-chairperson of the Hochschulrat (supervisory board) of the RWTH Aachen University (Germany)
- 2000 - 2008, Member of the advisory board of ABINIT (open source electronic structure project, `www.abinit.org`)
- Organization, or member of scientific board, of several international workshops

National (France):

- 2009 - 2012, Nominated member of the Comité National CNRS (Section 06 Condensed Matter, Structures and Electronic Properties): recruitment of permanent researchers and evaluation of researchers and research unit projects of the CNRS on a national level
- 2000 - 2008, Member of the piloting board ("bureau") of the "Groupement de Recherche" (national research network) GDR "DFT" and "DFT++"
- Member of the "Comité Thématique Objets individuels/Composants élémentaires" for the Nanoscience program 2003 of the French Ministery of Research

Reviewing:

- Referee for international journals: Phys. Rev. Letters, Phys. Rev. B, Europhys. Letters, Surface Science, Nature Physics, Journal of Chemical Physics, *et c.*
- Reviewer in the French context, mainly: national science foundation Agence Nationale de la Recherche (ANR), regional (IledeFrance), supercomputing projects till 2007
- Reviewer for national science foundations other than French: European Science Foundation, Fonds zur Foerderung der wissenschaftlichen Forschung (Austrian Science Foundation), NSF USA, numerous punctual activities for Universities or supercomputing centres abroad.

Teaching and training:

- Invited teaching at summer schools at least once per year
- Lectures in the framework of the ETSF. Example: "Computational methods for timedependent many-electron systems", 3 days teaching with two other group members, Queen's University Belfast.

Awards and Fellowships

- Fellow of the American Physical Society (2007)
- CNRS Silver Medal (2003)
- Marie Curie Individual European Fellowship (1991-1992)
- Supported by Carl Duisberg Stiftung, Bayer industries (1987)
- Supported by the Studienstiftung des Deutschen Volkes, Federal German foundation for the support of outstanding students (University: 1981-1986 and PhD: 1988-1990)

Society

- Contributions to questions of women and men in society, e.g. in the film "femmes de tête", 29.6.2004 on ARTE, `herve.nisic.free.fr/femmes.de.tete/fdt.html`, or exhibition "physique de femmes", `www2.cnrs.fr/sites/communique/fichier/panneaux_fin.pdf`
- Vocational Guidance Day at the Franco-German Highschool of Buc (France): presentation of the job of physicist in academic research, since 2004

Publications (about 3600 citations, h-index = 30)

[1] G. Lani, P. Romaniello, and L. Reining, "Approximations for many-body green's functions: insights from the fundamental equations," New Journal of Physics **14**, 013056 (2012), URL `http://stacks.iop.org/1367-2630/14/i=1/a=013056`.

[2] M. Guzzo, G. Lani, F. Sottile, P. Romaniello, M. Gatti, J. J. Kas, J. J. Rehr, M. G. Silly, F. Sirotti, and L. Reining, "Valence electron photoemission spectrum of semiconductors: *Ab Initio* description of multiple satellites," Phys. Rev. Lett. **107**, 166401 (2011), URL `http://link.aps.org/doi/10.1103/PhysRevLett.107.166401`.

[3] M. A. L. Marques, J. Vidal, M. J. T. Oliveira, L. Reining, and S. Botti, "Density-based mixing parameter for hybrid functionals," Phys. Rev. B **83**, 035119 (2011).

[4] M. Cazzaniga, H.-C. Weissker, S. Huotari, T. Pylkkänen, P. Salvestrini, G. Monaco, G. Onida, and L. Reining, "Dynamical response function in sodium and aluminum from time-dependent density-functional theory," Phys. Rev. B **84**, 075109 (2011), URL http://link.aps.org/doi/10.1103/PhysRevB.84.075109.

[5] S. Huotari, M. Cazzaniga, H.-C. Weissker, T. Pylkkänen, H. Müller, L. Reining, G. Onida, and G. Monaco, "Dynamical response function in sodium studied by inelastic x-ray scattering spectroscopy," Phys. Rev. B **84**, 075108 (2011), URL http://link.aps.org/doi/10.1103/PhysRevB.84.075108.

[6] I. Aguilera, J. Vidal, P. Wahnón, L. Reining, and S. Botti, "First-principles study of the band structure and optical absorption of cugas2," Phys. Rev. B **84, 085145** (2011), URL http://link.aps.org/doi/10.1103/PhysRevB.84.085145.

[7] J. A. Berger, L. Reining, and F. Sottile, "Ab initio calculations of electronic excitations: Collapsing spectral sums," Phys. Rev. B **82**, 041103(R) (2010).

[8] H.-C. Weissker, J. Serrano, S. Huotari, E. Luppi, M. Cazzaniga, F. Bruneval, F. Sottile, G. Monaco, V. Olevano, and L. Reining, "Dynamic structure factor and dielectric function of silicon for finite momentum transfer: Inelastic x-ray scattering experiments and ab initio calculations," Phys. Rev. B **81**, 085104 (2010), URL http://prb.aps.org/abstract/PRB/v81/i8/e085104.

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[10] J. Vidal, S. Botti, P. Olsson, J.-F. Guillemoles, and L. Reining, "Strong interplay between structure and electronic properties in cuin(s,se)2: A first-principles study," Phys. Rev. Lett. **104**, 056401 (2010), URL http://link.aps.org/doi/10.1103/PhysRevLett.104.056401.

[11] P. Romaniello, D. Sangalli, J. A. Berger, F. Sottile, L. G. Molinari, L. Reining, and G. Onida, "Double excitations in finite systems," Journal of Chemical Physics **130**, 044108 (2009), URL http://dx.doi.org/10.1063/1.3065669.

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Invited talks and invited lectures given by myself since 1996

[1] Correlation: coupling of excitations. In *Workshop "Strong Correlation from First Principles (SC1p)", Kloster Seeon, Germany*, 08/30-09/2 2011.

[2] Density functionals from many-body perturbation theory: some thoughts. In *CECAM workshop on "How to Speed up Progress and Reduce Empiricism in Density Functional Theory", ACAM Dublin, Ireland*, 06/20-24 2011.

[3] Insight and prediction of materials properties from ab initio calculations of electronic excitations. In *Workshop on Dynamics, Properties, and Solidification of Liquid Alloys, German Aerospace Center, Cologne, Germany*, 07/7-9 2011.

[4] Satellite structure in electronic spectra. In *ES11: The 23rd Annual Workshop on Electronic Structure Methods, University of Pennsylvania, USA*, 06/6-9 2011. together with the participation in a panel discussion about ways to organize collaboration within the electronic structure community.

[5] Bethe salpeter & gw. In *DoE Workshop Theories of Excited States in Molecules and Nanostructures, Baltimore (USA)*, 06/13-14 2010.

[6] Many-body approaches. In *International Summer School on Electronic Structure Theory and Materials Design, Copenhagen (Denmark)*, 08/14-20 2010.

[7] Many-body perturbation theory: from fundamental ideas to use in practice. In *CECAM-Tutorial "HoW exciting! - Hands-on workshop on excitations in solids employing the EXC! TiNG code", Lausanne (Switzerland)*, 11/11-17 2010.

[8] Overview of rpa from the condensed matter perspective. In *Multidisciplinary Workshop on RPA, Paris (France)*, 01/26-29 2010.

[9] Overview on scgf methods in electronic systems. In *Self-consistent Green's function methods: From solid state to nuclear physics: modern challenges and bridging to energy density functionals, Saclay (France)*, 09/09-10 2010.

[10] Correlation in electronic excitations. In *14th International Workshop on Computational Physics and Materials Science, Trieste (Italy)*, 01/08-10 2009.

[11] Electronic response - theoretical approaches and link to experiment. In *Workshop Understanding Materials through Electron Microscopes - Realising the Potential, London (United Kingdom)*, 04/22-24 2009.

[12] Insight and prediction of material properties from ab initio calculations of electronic excitations. In *Symposium Ab-initio approaches to excitations in condensed matter at DPG spring meeting, Dresden (Germany)*, 03/25-27 2009.

[13] Insight and prediction of materials properties from ab initio calculations of electronic excitations. In *OSI-VIII Optic of surfaces and interfaces VIII*, 09/07-11 2009.

[14] Many-body perturbation theory: approaches and applications, limitations and good news. In *KITP workshop From Basic Concepts to Real Materials, Santa Barbara (USA)*, 11/02-06 2009.

[15] Ab initio calculations of electronic response - ingredients, results and challenges. In *Workshop Recent Developments in Electronic Structure, University of Illinois Urbana (USA)*, 06 2008.

[16] Electronic response: theoretical approaches and link to experiment. In *MORE: Meeting on Optical Response in Extended Systems, Vienna (Austria)*, 11/19-21 2008.

[17] Exchange and correlation effects in electronic spectra: contributions from ab initio calculations. In *Workshop on X-ray spectroscopies: theory and experiment, Lausanne (Switzerland)*, 01 2008.

[18] Insight and prediction of material properties from ab initio calculations of electronic excitations. In *Second International Symposium on Structure-Property Relationships in Solid State Materials, Nantes (France)*, 06 2008.

[19] Electronic response: theoretical approaches and link to experiment. In *SFB (German research fund) in semi-conductor physics meeting, Würzburg (Germany)*, 07 2007.

[20] How to combine the reliability of manybody perturbation theory and the efficiency of tddft? context, possibilities and applications. In *deMon developpers meeting, Paris (France)*, 09 2007.

[21] How to get just the information you want - from many-body perturbation theory to timedependent density functional theory, and other shortcuts. In *Gordon Research Conference on Time-Dependent Density-Functional Theory, Waterville (USA)*, 07 2007.

[22] Many-body perturbation theory and density-functional based approaches: successful combinations. In *APS March meeting, Denver (USA)*, 03 2007.

[23] Many-body perturbation theory and density-functional based approaches: successful combinations. In *Third International Workshop on DFT applied to metals and alloys, Oran (Algeria)*, 05 2007.

[24] Many-body perturbation theory and density-functional based approaches: successful combinations. In *DFT2007 conference on the Theory and Applications of DFT, Amsterdam (Netherlands)*, 08 2007.

[25] Beyond the gw approximation. In *Workshop Recent developments in computational electronic structure, Cambridge (United Kingdom)*, 01 2006.

[26] Beyond the gw approximation. In *Workshop First principles approaches to optical and photoelectron spectra, München (Germany)*, 03 2006.

[27] Beyond the gw approximation. In *International Workshop on First Principles Calculation of Correlated Electrons, Tokyo (Japan)*, 11-12 2006.

[28] The inverse dielectric function - theoretical approaches and contributions to theory from experiment. In *DFTEM 2006, Vienna (Austria)*, 04 2006.

[29] La fonction diélectrique inverse: comment la calculer, comment l'utiliser ? In *Workshop JEELS 06, Blois (France)*, 05 2006.

[30] Many-body perturbation theory and density-functional approaches: successful combinations. In *Workshop Applications of the Bethe-Salpeter Equation, Houffalize (Belgium)*, 09 2006.

[31] Many-body versus tddft. In *School TDDFT, Benasque (Spain)*, 09 2006.

[32] Towards a european theoretical spectroscopy facility: research is collaboration. In *Workshop Nanocose 3, Rome (Italy)*, 10 2006.

[33] Dft - fonctionnelles. In *School DFT, Caen (France)*, 06 2005.

[34] Electronic excitations and the calculation of dielectric functions. In *Satellite workshop of the Users meeting ELETTRA, Trieste (Italy)*, 12 2005.

[35] Electronic excitations and the calculation of dielectric functions. In *Workshop synchrotron SOLEIL Spectroscopies d'électrons et diffusion inélastique en matière condensée : vers une meilleure compréhension des effets de corrélation, Saint Aubin (France)*, 11 2005.

[36] Electronic excitations and the calculation of dielectric functions. In *Wissenschaftskolleg "Computational Materials Science", Vienna (Austria)*, 10 2005.

[37] Electronic excitations: bandstructure and many-body effects. In *Wissenschaftskolleg "Computational Materials Science", Vienna (Austria)*, 10 2005.

[38] Electronic excitations in tddft and in many-boby perturbation theory: comparisons and combinations. In *ICTP INFM-DEMOCRITOS ISMO - IUT School and workshop on Electronic-structure calculations and their applications in materials science, Isfahan (Iran)*, 05 2005.

[39] How to describe exchange and correlation effects in the response properties of valence electrons? In *ICTP INFM-DEMOCRITOS ISMO - IUT School and workshop on Electronic-structure calculations and their applications in materials science, Isfahan (Iran)*, 05 2005.

[40] Many-boby perturbation theory using the density-functional concept: a successful combination! In *Conference Excited-state properties of solids , Mannheim (Germany)*, 05 2005.

[41] Many-boby perturbation theory using the density-functional concept: a successful combination! In *Workshop Orbital Functionals for Exchange and Correlation: the optimized effective potential and related methods, Berlin (Germany)*, 03 2005.

[42] Theoretical spectroscopy: some developments and applications based on gw. In *Workshop 40 years of the GW approximation for the Electronic Self-Energy: Achievements and Challenges , Bad Honnef (Germany)*, 09 2005.

[43] Ab initio calculations of electronic excitations: challenges and recent progress. In *E-MRS meeting, Strasbourg (France)*, 05 2004.

[44] Ab initio theory of electronic excited states. In *INFM meeting, Genova (Italy)*, 06 2004.

[45] How to describe exchange and correlation effects in the response properties of valence electrons? answers from tddft and many-boby perturbation theory. In *Workshop and School Time-Dependent Density-Functional Theory: Prospects and Applications , Benasque (Spain)*, 08-09 2004.

[46] How to describe exchange and correlation effects in the response properties of valence electrons? In *APS March Meeting, Montreal (Canada)*, 03 2004.

[47] Tddft and many-boby perturbation theory: comparisons and combinations. In *Workshop Theory and Modeling of Electronic Excitations in Nanoscience , Maratea (Italy)*, 09 2004.

[48] Tddft and many-boby perturbation theory: comparisons and combinations. In *Workshop and School Time-Dependent Density-Functional Theory: Prospects and Applications , Benasque (Spain)*, 08-09 2004.

[49] Electron-hole excitations in the quasipinproceedings and in the density-functional framework. In *Workshop Computational Materials Science, Cagliari (Italy)*, 09 2003.

[50] Electron-hole excitations in the quasipinproceedings picture and in the density-functional framework. In *XITH Int. Workshop of Computational Physics and Material Science, Trieste (Italy)*, 01/16-18 2003.

[51] Electron-hole excitations in the quasipinproceedings picture and in the density-functional framework. In *Sanibel Symposium, University of Florida Quantum Theory Project (USA)*, 02/22-03/01 2003.

[52] Recent progress in developments and applications of time-dependent density functional theory. In *Workshop Computational Materials Science, Cagliari (Italy)*, 09 2003.

[53] Self-consistent electronic response in the quasipinproceedings and in the density-functional framework. In *EXCITING RTN workshop in Louvain-La-Neuve (Belgium)*, 04/14-16 2003.

[54] Calculs des spectres electroniques: quelle reponse ? In *JMC8, Marseille (France)*, 08/27-30 2002.

[55] Effects of long-range interactions in the absorption and loss spectra of finite and infinite systems. In *International workshop Total energy methods in computational condensed matter , Tenerife (Spain)*, 01 2002.

[56] Etudes théoriques des propriétés optiques de surface. In *Journées Surface/Interface, Rennes (France)*, 01 2001.

[57] Exchange and correlation treated using the gw and bethe-salpeter approaches for the calculation of excited states. In *CECAM workshop Electronic properties of strongly correlated systems, Lyon (France)*, 07 2001.

[58] Ab-initio theory of optical properties. In *INFM meeting 2000, Genova (Italy)*, - 2000.

[59] Application of green's functions methods to the calculation of excited states. In *PSIK 2000 conference, Schwaebisch Gmuend (Germany)*, 08 2000.

[60] Application of green's functions methods to the calculation of optical properties. In *APS 2000 march meeting, Minneapolis (USA)*, - 2000.

[61] The calculation of electronic excitations : some recent developments. In *Workshop on Excited State Properties and Response Functions for Materials , Minneapolis (USA)*, 11 2000.

[62] Introduction to the calculation of many-body effects in eel spectra. In *Meeting Challenges in ELNES, Paris (France)*, 09 2000.

[63] Ab initio calculation of response properties including the electron-hole interaction. In *MRS Fall meeting, Boston (USA)*, 11/29-12/2 1999.

[64] Some remarks about the ab initio calculation of local field and excitonic effects in the dielectric function. In *Ninth International Workshop on Computational Materials Science: Electronic Structure Theory and Simulations, Trieste (Italy)*, 01/14-16 1999.

[65] Ab initio calculation of excitons. In *International workshop on Large Scale Quantum Simulations: Total Energy and Force Methods, Tsukuba (Japan)*, 01/12-14 1998.

[66] Calculs de structure de bandes. In *Journées EELS : Spectrométrie de pertes d'énergie d'électrons, Gruissan (France)*, 10/5-7 1998.

[67] Excitonic effects in the optical properties. In *Workshop EPIOPTICS 5, Erice (Italy)*, 06/17-22 1998.

[68] First principles calculations of photoemission spectra in clusters. In *CECAM meeting EXCAM, Lyon (France)*, 09/11-12 1998.

[69] Ab initio calculation of excitons. In *CECAM workshop Excited electrons in molecules, solids and atoms, Lyon (France)*, 09/8-10 1997.

[70] Spectroscopie électronique des matériaux: calculs ab-initio des états excités. In *5ème journées de la matière condensée (SFP), Orléans (France)*, - 1996.

Languages

Professional in German, French, Italian, English