Guido ROMA
born in Modena (Italy), 11/2/1966
married, two children

Studies and diplomas

29.05.2012 *Habilitation à Diriger des Recherches*. Université Pierre et Marie Curie, Paris, France.

12.1992-11.1995 PhD (*Dottorato*) in physics. University of Rome *Tor Vergata*.
Date of examination: 11.10.1996

12.1991-11.1992 National service: civil servant at a music library

1985-1991 Graduation (*Laurea*) *in Physics. University of Modena, Italy. Final mark: 109/110. Date of examination: 25.07.1991*

1979-1984 Classical Lycæum *L.A. Muratori* Modena (Italy).
Diploma: *Maturità*, Final mark: 55/60.

Professional records

05.2014 - present back again at CEA/SRMP as permanent staff

05.2013 - 04.2014 Research associate, Johannes Gutenberg University, Mainz, Germany (on Sabbatical leave from CEA Saclay - France)

05.2011 - 04.2013 Visiting scientist at Johannes Gutenberg University, Mainz, Germany

10.2001 - 04.2013 Researcher (permanent staff) at CEA (Commissariat à l'Énergie Atomique), Service de Recherches de Métallurgie Physique (SRMP), Saclay, France.

08.2000 - 10.2001 Researcher (fixed term) at CEA (Commissariat à l'Énergie Atomique), Service de Recherches de Métallurgie Physique (SRMP), Saclay, France.

01.1997 - 07.2000 Post-doctoral researcher and system administrator at Centre Européen de Calcul Atomique et Moléculaire (CECAM) - Lyon, France.

06.1996-12.1996 Travel Grant by the University of Modena to work at Centre Européen de Calcul Atomique et Moléculaire (CECAM) - Lyon, France.

04.1996-05.1996 Research contract with INFM (Italian National Institute for the Physics of Matter), at the University of Modena, Italy.

Scientific subjects

Keywords: First principles calculations, defects, diffusion, irradiation effects, electronic structure, phonons, surfaces, photovoltaics.

First principles calculations of defects and diffusion properties

I have been involved for several years in the study of defects and diffusion in non-metallic materials, as the basic phenomena for the understanding of non-equilibrium kinetic processes controlling the modifications of materials induced by irradiation of different nature (neutrons, charged ions, electrons, X/Gamma). I investigate these phenomena by computer simulation at the atomic scale based on a quantum description, coupled with models at higher scales. I have focused in particular on silicon carbide and silicon dioxide, two materials of interest for nuclear applications, but also two prototypical materials (a wide band gap semiconductor and an amorphous insulating oxide), of crucial importance in the semiconductor industry and for several other applications. Notable contributions of my work include insights into oxygen and silicon self-diffusion mechanisms in silicon dioxide and into a variety of kinetic mechanisms and defects in silicon carbide, including impurity diffusion.

More recently I started projects on defects and impurities in boron carbide, a material with a complex structure and still not fully understood, and on chemical defects in polyethylene, opening the Pandora's jar of polymers and organic materials.

Since 2011 I have enlarged the scope of my research to materials for photovoltaic applications, again with a focus on point defects, but also on surface thermodynamics and kinetics. In this respect, I was involved in a project devoted to computer simulation of atomic processes at surfaces and interfaces in thin films solar cells based on chalcopyrite quaternary semiconductors $CuIn_xGa_{1-x}Se_2$ (CIGS). In the last few years I devoted part of my time to halide perovskite materials for solar cells, in particular $CsPbI_3$, with special attention to phonon instabilities, phase stability and their influence on the electronic properties, including spin related properties like the Rashba effect and ferroelectricity.

Other fields of interest

Layered materials (graphite, TM di-chalcogenides, intercalation compounds)

Ab-initio phonons

Nanostructures

Surface thermodynamics and kinetics

Irradiation effects

Photovoltaics

Publications

Regular Papers

1. Muriel Ferry, Yunho Ahn, Florian Le Dantec, Yvette Ngono, and Guido Roma. Combining experimental and theoretical tools to probe radio-oxidation products in polyethylene. *Polymers*, 15:1537, 2023

2. Yunho Ahn, Guido Roma, and Xavier Colin. Elucidating the role of alkoxy radicals in polyethylene radio-oxidation kinetics. *Macromolecules*, 55(19):8676–8684, 2022

3. Guido Roma, Antoine Jay, Nathalie Vast, Olivier Hardouin Duparc, and Gaëlle Gutierrez. Reply to "comment on 'understanding first-order raman spectra of boron carbides across the homogeneity range' ". *Phys. Rev. Materials*, 6:016602, Jan 2022

4. Yunho Ahn, Xavier Colin, and Guido Roma. Atomic scale mechanisms controlling the oxidation of polyethylene: A first principles study. *Polymers*, 13(13):2143, 2021

5. Guido Roma, Kevin Gillet, Antoine Jay, Nathalie Vast, and Gaëlle Gutierrez. Understanding first-order Raman spectra of boron carbides across the homogeneity range. *Phys. Rev. Materials*, 5:063601, Jun 2021

6. Guido Roma, Arthur Marronnier, and Jacky Even. From latent ferroelectricity to hyperferroelectricity in alkali lead halide perovskites. *Phys. Rev. Materials*, 4:092402 (R), Sep 2020

7. Arthur Marronnier, Guido Roma, Marcelo A. Carignano, Yvan Bonnassieux, Claudine Katan, Jacky Even, Edoardo Mosconi, and Filippo De Angelis. Influence of Disorder and Anharmonic Fluctuations on the Dynamical Rashba Effect in Purely Inorganic Lead-Halide Perovskites. *J. Phys. Chem. C*, 123:291–298, 2019

8. Kevin Gillet, Guido Roma, Jean-Paul Crocombette, and Dominique Gosset. The influence of irradiation induced vacancies on the mobility of helium in boron carbide. *J. Nucl. Mater.*, 512:288–296, 2018

9. Arthur Marronnier, Guido Roma, Soline Boyer-Richard, Laurent Pedesseau, Jean-Marc Jancu, Yvan Bonnassieux, Claudine Katan, Constantinos C. Stoumpos, Mercouri G. Kanatzidis, and Jacky Even. Anharmonicity and disorder in the black phases of cesium lead iodide used for stable inorganic perovskite solar cells. *ACS Nano*, 12(4):3477–3486, 2018

10. Guido Roma, Fabien Bruneval, and Layla Martin-Samos. Optical properties of saturated and unsaturated carbonyl defects in polyethylene. *J. Phys. Chem. B*, 122:2023–2030, 2018

11. Arthur Marronnier, Heeryung Lee, Heejae Lee, Minjin Kim, Céline Eypert, Jean-Paul Gaston, Guido Roma, Denis Tondelier, Bernard Geffroy, and Yvan Bonnassieux. Electrical and optical degradation study of methylammonium-based perovskite materials under ambient conditions. *Solar Energy Materials and Solar Cells*, 178:179 – 185, 2018

12. Anton Schneider, Guido Roma, Jean-Paul Crocombette, Vianney Motte, and Dominique Gosset. Stability and kinetics of helium interstitials

in boron carbide from first principles. *Journal of Nuclear Materials*, 496(Supplement C):157 – 162, 2017

13. Arthur Marronnier, Heejae Lee, Bernard Geffroy, Jacky Even, Yvan Bonnassieux, and Guido Roma. Structural instabilities related to highly anharmonic phonons in halide perovskites. *The Journal of Physical Chemistry Letters*, 8:2659–2665, 2017

14. Hossein Mirhosseini, Janos Kiss, Guido Roma, and Claudia Felser. Reducing the Schottky barrier height at the $MoSe_2$/Mo(110) interface in thin-film solar cells: insights from first-principles calculations. *Thin Solid Films*, 606:143–147, 2016

15. Elaheh Ghorbani, Janos Kiss, Hossein Mirhosseini, Guido Roma, Markus Schmidt, Johannes Windeln, Thomas D. Kühne, and Claudia Felser. Hybrid-Functional Calculations on the Incorporation of Na and K Impurities into the $CuInSe_2$ and $CuIn_5Se_8$ Solar-Cell Materials. *J. Phys. Chem. C*, 119(45):25197–25203, 2015

16. Hossein Mirhosseini, Guido Roma, Janos Kiss, and Claudia Felser. First-principles investigation of the bulk and low-index surfaces of $MoSe_2$. *Phys. Rev. B*, 89:205301, 2014

17. Guido Roma, Elaheh Ghorbani, Hossein Mirhosseini, Janos Kiss, Thomas D. Kühne, and Claudia Felser. Predicting the stability of surface phases of molybdenum selenides. *Appl. Phys. Lett.*, 104:061605, 2014

18. Janos Kiss, Thomas Gruhn, Guido Roma, and Claudia Felser. Theoretical Study on the Diffusion Mechanism of Cd in the Cu-Poor Phase of $CuInSe_2$ Solar Cell Material. *J. Phys. Chem. C*, 117:25933–25938, 2013

19. Guido Roma and Letizia Chiodo. Selenium adsorption on Mo(110): A first-principles investigation. *Phys. Rev. B*, 87:245420, 2013

20. Janos Kiss, Thomas Gruhn, Guido Roma, and Claudia Felser. Theoretical Study on the Structure and Energetics of Cd Insertion and Cu Depletion of $CuIn_5Se_8$. *J. Phys. Chem. C*, 117(21):10892–10900, 2013

21. Fabien Bruneval and Guido Roma. Energetics and metastability of the silicon vacancy in cubic SiC. *Phys. Rev. B*, 83:144116, 2011

22. Ting Liao, Olga Natalia Bedoya-Martínez, and Guido Roma. Stoichiometric defects in silicon carbide. *J.Phys. Chem. C*, 114:22691–22696, 2010.

23. Olga Natalia Bedoya-Martínez and Guido Roma. Activation entropies for diffusion in cubic silicon carbide from first principles. *Phys. Rev. B*, 82:134115, 2010.

24. G. Roma and J.-P. Crocombette. Evidence for a kinetic bias towards antisite formation in SiC nano-decomposition. *J. Nucl. Mater.*, 403:32–41, 2010.

25. L. Martin-Samos, G. Roma, P. Rinke, and Y. Limoge. Charged oxygen defects in SiO_2: going beyond local and semilocal approximations to density functional theory. *Phys. Rev. Lett.*, 104:075502, 2010.

26. G. Roma. Palladium in cubic silicon carbide: stability and kinetics. *J. Appl. Phys.*, 106:123504, 2009.

27. T. Liao, G. Roma, and J. Y. Wang. Neutral silicon interstitials in 3C and 4H silicon carbide: a first principles study. *Philos. Mag.*, 89:2271–2284, 2009.

28. L. Martin-Samos, Y. Limoge, and G. Roma. Defects in amorphous SiO_2: Valence alternation pair model. *Phys. Rev. B*, 76:104203, 2007.

29. L. Martin-Samos, Y. Limoge, J. P. Crocombette, G. Roma, N. Richard, E. Anglada, and E. Artacho. Neutral self-defects in a silica model: A first-principles study. *Phys. Rev. B*, 71:014116, 2005.

30. L. Martin-Samos, Y. Limoge, N. Richard, J. P. Crocombette, G. Roma, E. Anglada, and E. Artacho. Oxygen neutral defects in silica: Origin of the distribution of the formation energies. *Europhys. Lett.*, 66:680–686, 2004.

31. G. Roma and Y. Limoge. Density functional theory investigation of native defects in SiO_2: Self-doping and contribution to ionic conductivity. *Phys. Rev. B*, 70:174101, 2004.

32. G. Roma, Y. Limoge, and S. Baroni. Oxygen self-diffusion in α-quartz. *Phys. Rev. Lett.*, 86:4564–4567, 2001.

33. S. Ossicini, C. M. Bertoni, M. Biagini, A. Lugli, G. Roma, and O. Bisi. Optical properties of isolated and interacting silicon quantum wires. *Thin Solid Films*, 297:154–162, 1997.

34. G. Roma, C. M. Bertoni, and S. Baroni. The phonon spectra of LiH and LiD from density-functional perturbation theory. *Sol. State Commun.*, 98:203–207, 1996.

Conference proceedings (reviewed)

35. G. Roma. Modelling the contribution of point defects to the raman spectrum of crystalline materials. *Modelling Simul. Mater. Sci. Eng.*, 27:074001, 2019

36. Guido Roma. Linear response calculation of first-order raman spectra of point defects in silicon carbide. *physica status solidi (a)*, 213:2995, 2016

37. Ting Liao and Guido Roma. First principles defect energetics for simulations of silicon carbide under irradiation: Kinetic mechanisms of silicon di-interstitials. *Nucl. Instrum. Meth. Phys. Res. B*, 327:52–58, 2014

38. Guido Roma, Fabien Bruneval, Ting Liao, Olga Natalia Bedoya Martínez, and Jean-Paul Crocombette. Formation and migration energy of native defects in silicon carbide from first principles: an overview. *Def. Diff. Forum*, 323-325:11, 2012.

39. Guido Roma. The influence of palladium impurities on vacancy diffusion in cubic silicon carbide. In J.K. Gibson, S.K. McCall, E.D. Bauer, L. Soderholm, T. Fanghaenel, R. Devanathan, A. Misra, C. Trautmann, and B.D. Wirth, editors, *Basic Actinide Science and Materials for Nuclear Applications*, volume 1264 of *Mater. Res. Soc. Proc.*, 2010.

40. T. Liao and G. Roma. Stability of neutral silicon interstitials in 3C- and 4H-SiC: A first-principles study. *Def. Diff. Forum*, 283-286:74–83, 2009.

41. Guido Roma, Yves Limoge, and Layla Martin-Samos. Oxygen and silicon self-diffusion in quartz and silica: The contribution of first principles calculations. *Def. Diff. Forum*, 258-260:542–553, 2006.

42. Guido Roma, Yves Limoge, and Layla Martin-Samos. Aspects of point defects energetics and diffusion in SiO_2 from first principles simulations. *Nucl. Instrum. Meth. Phys. Res. B*, 250:54–56, 2006.

43. G. Roma and Y. Limoge. First principles suggestions of targeted diffusion experiments on SiO_2. *Def. Diff. Forum*, 237-240:127–132, 2005.

44. N. Richard, L. Martin-Samos, G. Roma, Y. Limoge, and J. P. Crocombette. First principle study of neutral and charged self-defects in amorphous SiO_2. *J. Non-Cryst. Solids*, 351:1825–1829, 2005.

45. L. Martin-Samos, Y. Limoge, J. P. Crocombette, G. Roma, and N. Richard. Oxygen self-diffusion mechanisms in silica by first-principles. *Def. Diff. Forum*, 237-240:115–120, 2005.

46. G. Roma and Y. Limoge. A first principles study of native defects in α-quartz. *Nucl. Instrum. Meth. Phys. Res. B*, 202:120–124, 2003.

47. G. Roma, Y. Limoge, and S. Baroni. Oxygen self-diffusion in SiO_2: An ab-initio approach. *Def. Diff. Forum*, 194-1:287–293, 2001.

48. S. Ossicini, M. Biagini, C. M. Bertoni, G. Roma, and O. Bisi. Ab-initio calculation of the optical properties of silicon quantum wires. In Robert W. Collins, Philippe M. Fauchet, Isamu Shimizu, Jean-Claude Vial, Toshikazu Shimada, and A. Paul, editors, *Advances in Microcrystalline and Nanocrystalline Semiconductors – 1996*, volume 452 of *Mater. Res. Soc. Proc.*, pages 63–68, Pittsburgh, PA, 1997.

Other conference proceedings

49. Arthur Marronnier, Guido Roma, Soline Boyer-Richard, Laurent Pedesseau, Yvan Bonnassieux Jean-Marc Jancu, Claudine Katan, Constantinos C. Stoumpos, Mercouri Kanatzidis, and Jacky Even. Anharmonicity and Disorder in the Black Phases of CsPbI3 used for Stable Inorganic Perovskite Solar Cells. In *Proceedings of the 2018 WCPEC-7 (PVSC-45),*, 2018

50. Guido Roma, Letizia Chiodo, and Janos Kiss. Adsorption of Se, Na, and O on the Mo(110) surface: modeling atomic mechanisms at the back contact of thin film chalcopyrite solar cells. In *2013 IEEE 39th Photovoltaic Specialists Conference (PVSC 2013)*, page 3300. Institute of Electrical and Electronics Engineers (IEEE), Apr 2014

51. Janos Kiss, Guido Roma, and Claudia Felser. Theoretical Study of Zn and Cd Interstitials and Substitutional Interstitials in $CuInSe_2$ via

Hybrid Functional Calculations. In *2013 IEEE 39th Photovoltaic Specialists Conference (PVSC2013)*, page 1983. Institute of Electrical and Electronics Engineers (IEEE), Apr 2014

52. G. Roma, L. Martin-Samos, P.Rinke, and Y. Limoge. Modélisation "ab-initio" des défauts dans les isolants : SiO_2 comme un cas test de la validité des approches DFT et GW. In *Actes du Colloque Matériaux 2010, 18-22 Octobre, Nantes*, 2010. CDROM

53. Guido Roma. A first principles study of palladium impurities in silicon carbide. *Adv. Sci. Technol.*, 45:1969–1973, 2006

54. S. Ossicini, M. Biagini, C. M. Bertoni, G. Roma, and O. Bisi. Confinement and passivation in isolated and coupled silicon quantum wires. In M. Scheffler and R. Zimmermann, editors, *23rd International Conference on the Physics of Semiconductors*, pages 1205–1208, Berlin, Germany, July 1996. World Scientific

Articles in books

55. Muriel Ferry, Guido Roma, Florence Cochin, Stéphane Esnouf, Vincent Dauvois, Fidèle Nizeyimana, Benoit Gervais, and Yvette Ngono-Ravache. 3.16 - polymers in the nuclear power industry. In Rudy J.M. Konings and Roger E. Stoller, editors, *Comprehensive Nuclear Materials (Second Edition)*, pages 545 – 580. Elsevier, Oxford, second edition edition, 2020

56. Guido Roma, Fabien Bruneval, and Jean-Paul Crocombette. Structure et cinétique des défauts ponctuels dans le carbure de silicium. In *Les matériaux du nucléaire : Modélisation et simulation des matériaux de structure*, Monographies de la Direction de l'Énergie Nuclléaire. Editions Le Moniteur, 2016

57. C. M. Bertoni, G. Roma, and R. Di Felice. Electronic structure of adsorbates on surfaces. Adsorption on semiconductors. In M. Scheffler and K. Horn, editors, *Electronic Structure*, volume II of *Handbook of Surface Science*, pages 247–283. Elsevier Science B. V., The Netherlands, 2000.

Conference presentations

Several presentations at international conferences (> 30) since 1996, including MRS (Fall meeting 2001, 2008, Spring meeting 2007, 2010), DIMAT

(2000,2004,2008), MMM (2006, 2014, 2016, 2018), CIMTEC(2006), IEEE-Photovoltaic Specialists Conference (2013), ICDIM(2016), DPG Spring Meeting (2014, 2017, 2018), TMS (2021).

Invited talks at a CECAM workshop in 2002, DSL conference (Diffusion in solids and liquids) in 2006,2007,2008, DIMAT conference (DIffusion in MATerials) 2011 (plenary talk), EMN (Energy, Materials, Nanotechnology) Spring meeting (Orlando, USA, 4/2013), E-MRS meeting (Strasbourg, France, 5/2013), PACRIM (Waikoloa, HI, USA, 5/2017).

Tutoring

Tutoring or co-tutoring of graduate students (8), PhD Students (8), postdocs (2) in France and in Germany.

Other skills and recognitions

- Refereeing activity for the following journals:

  Physical Review Letters, Nature Communications, Physical Review B, Physical Review Materials, Journal of Applied Physics, Applied Physics Letters, ACS Applied Materials & Interfaces, ACS Applied Energy Materials, ACS Energy Letters, Defects and Diffusion Forum, Nuclear Instruments and Methods in Physical Research , Zeitschrift für Physikalische Chemie, Physica Status Solidi, Computational Materials Science, Journal of Nuclear Materials, Acta Materialia, Inorganic Chemistry, Current Opinion in Solid State & Materials Science, Magnetism and Magnetic Materials.

- 2020-2023: ANR funding for projet TRAPPER

- 2017-2021: EU-H2020 funding for project TeaM Cables

- 2013-2014: PRACE-DECI computing time allocation (PI of project NaUSIKAS)

- 2013-2014: Funding from project comCIGS II on thin film photovoltaics, supported by the German Ministery of Environment

- 18.12.2015: named *CEA senior expert* (Materials Science, Solid State and Semiconductor Physics)

- Grants from EFDA (European Fusion Development Agreement) in 2008, 2009, and 2010 (32k€, 142k€, 142k€ in baseline support).

- 01.01.2010: named *CEA expert* (Materials Science, Solid State and Semiconductor Physics)
- Qualification as lecturer ("Maître de Conférence") obtained in 2001 from the French University Committee (Section: Chemistry of solids).

High Performance Computing : vector and massively parallel calculations

- CEA-DEN representative at the user group of CCRT computing center (2002-2011)
- In charge of a tender for buying a 200 kEuro cluster in 2007

UNIX system administration

Workshop co-organisation

Written and oral skills in english, french, italian; german intermediate level.