Giacomo GIORGI

Dept. of Civil & Environmental Engineering (DICA).
The University of Perugia,
Via Duranti, 93
I-06125, Perugia, ITALY.

giacomo.giorgi@unipg.it
+39–075–585–3836

ACADEMIC EXPERIENCE

PRESENT POSITION

2016 Jan– ***Associate Professor (SSD: CHIM/07)*** c/o Department of Civil & Environmental Engineering (DICA). **The University of Perugia**, Italy.

PREVIOUS POSITIONS

2013 Aug– 2015 Dec ***Senior Researcher*** c/o Department of Chemical System Engineering, **The University of Tokyo**, Japan (Group Leader: Prof. Koichi Yamashita).

2012 Jun – 2013 Jul ***Project Assistant Professor*** c/o Research Center for Advanced Science and Technology (RCAST) – **The University of Tokyo**, Japan (Group Leader: Prof. Hiroshi Segawa)

2009 Feb – 2012 May *Post-Doctoral Fellow c/o* **The University of Tokyo**, Japan (Group Leader: Prof. Koichi Yamashita)

2008 Jan –Dec *Post-Doctoral Fellow*

The Institute of Molecular Science and Technologies (ISTM)

(Istituto di Scienze e Tecnologie Molecolari, **CNR-ISTM**, Perugia, Italy) c/o **The University of Perugia**, Italy.

"Electronic properties of complex molecular structures via ab-initio methods".

(Group Leader: Prof. Antonio Sgamellotti)

2007 Jan –Nov *Post-Doctoral Fellow* c/o

The University of Perugia, Italy.

Theoretical study of complex molecular systems (PRIN 2005 project: “Study and theoretical characterization of chemical species of interest in atmospheric processes” ("Studio e caratterizzazione teorica di specie chimiche di interesse nei processi atmosferici").
(Group Leader: Prof. Antonio Sgamellotti).

2005 Jan–2006 Dec *Post-Doctoral Fellow*

CONSORZIO CRESCI
(Centro per la Ricerca Eccellente per lo Sviluppo e per la Creazione d'Impresa). c/o **The University of Perugia**, Italy.

2004 Jan–2005 Jan *Post-Doctoral Fellow*

The Institute of Molecular Science and Technologies (ISTM)

(Istituto di Scienze e Tecnologie Molecolari, **CNR-ISTM**), Perugia, Italy c/o **The University of Perugia**, Italy.

Prototype study on a simulator of a solid state system in the field of Grid computing” ("Studio prototipale su un simulatore di un sistema allo stato solido nell'ambito del Grid-computing") involved in the FIRB project “Certified Platforms for highly performing computational grids oriented towards scalable virtual organizations” ("Piattaforme Abilitanti per Griglie Computazionali a Elevate Prestazioni Orientate a Organizzazioni Virtuali Scalabili"). (Dr. Francesco Mercuri)

FURTHER EXPERIENCE

2017 Feb Seminar activity; Research project development.

The University of Tokyo, Japan

(Group led by Prof. Hiroshi Segawa).

2008 Mar *Research fellow*

The University of Tokyo Japan

(Group Leader: Prof. Koichi Yamashita).

2006 Jun–Oct: *Research fellow*

The University of Tokyo, Japan.

(Group Leader: Prof. Koichi Yamashita).

EDUCATION

Oct 2000– Oct 2003	**PhD** in Chemical Sciences (XVI cycle) The University of Perugia, Italy PhD Thesis title: "Theoretical analysis of grafting and hydrosilylation process on silicon surfaces" (Discussed on Dec 04th 2003) Advisor: Prof. Antonio Sgamellotti.
Oct 1994–Nov1999	**M. Sc.** (laurea) in Chemistry, The University of Perugia, Italy. Laurea Thesis title: "Etching mechanisms on Si surfaces" (Discussed on Nov 15th 1999) Advisor: Prof. Antonio Sgamellotti.
1989–1994	Liceo Classico A. Mariotti (Perugia, Italy).

TEACHING EXPERIENCE

2019-2020	Class of Chemistry. Course: INDUSTRIAL ENGINEERING (Laurea - L08B - TERNI) The University of Perugia, Italy. Class of Chemistry. Course: BUILDING ENGINEERING & ARCHITECTURE (Laurea Magistrale Ciclo Unico 5 anni - MU07 - PERUGIA) The University of Perugia, Italy. (Co-teaching)
2018-2019	Class of Chemistry. Course: INDUSTRIAL ENGINEERING (Laurea - L08B - TERNI) The University of Perugia, Italy. Class of Chemistry. Course: BUILDING ENGINEERING & ARCHITECTURE (Laurea Magistrale Ciclo Unico 5 anni - MU07 - PERUGIA) The University of Perugia, Italy. (Co-teaching)
2017-2018	Class of Chemistry. Course: INDUSTRIAL ENGINEERING (Laurea - L08B - TERNI) The University of Perugia, Italy. Class of Chemistry. Course: BUILDING ENGINEERING & ARCHITECTURE (Laurea Magistrale Ciclo Unico 5 anni - MU07 - PERUGIA) The University of Perugia, Italy. (Co-teaching)
2016-2017	Class of Chemistry. Course: INDUSTRIAL ENGINEERING ([L-9] TERNI) The University of Perugia, Italy.

2018 Apr 04th	National Scientific Qualification ("Abilitazione Scientifica Nazionale") as **Full Professor**. Class 03/B2: "Fondamenti Chimici delle Tecnologie" (valid till 2024 Apr 6th)
2014 Feb 18th	National Scientific Qualification ("Abilitazione Scientifica Nazionale") as **Associate Professor**. Class 03/B2: "Fondamenti Chimici delle Tecnologie"
2012	Exercitations of Physical Chemistry. (Undergraduate students) Support to teaching (English language). The University of Tokyo, Japan.
2012	Material Simulation Course (Computational Packages for Theoretical Chemistry). Support to teaching (English language). The University of Tokyo, Japan
2009−2015	Tutorial activity of students of the University of Tokyo. PhD, BA, and MSc Students (H. Kawai, A. Kubo, T. Aoyama, Y. Masuda).

INSTITUTIONAL RESPONSABILITIES

2019- Member of the Docent College for the International PhD Course in "Civil and Environmental Engineering" of the University of Perugia, Italy (XXXV Cycle).

2019, Jan 23rd: PhD Final Exam External Examiner, The University of Bern, Switzerland (Candidate: Hassan Ouhbi)

04/09/2019 Reviewer for "Procedura dell'intervento FARE Ricerca in Italia: Framework per l'attrazione ed il rafforzamento delle eccellenze per la Ricerca in Italia". Assigned by MIUR (Italian Ministery for the University and Research, Dipartimento per la formazione e per la ricerca. Direzione Generale per il coordinamento, la promozione e la valorizzazione della Ricerca)

SERVICE

Reviewer for *Nature Comm., Acc. Chem. Res., ACS Energy Lett., ACS Nano, Scientific Reports, Nanoscale, Chem. Soc. Rev., J. Phys. Chem. Lett., J. Phys. Chem. C, Chem, Mater., Langmuir, PCCP, Computational Condensed Matter, Chem. Mater., RSC Advances, Chem. Phys. Lett., Solid State Communications, Nanotechnology, Physica Status Solidi B, Physica Status Solidi RRL, Phys. Lett. A, Chem. Lett., J. Amer. Chem. Soc., J. Mater Chem. A, J. Mater. Chem. C, Adv. Funct. Mater., APL Mater., Dyes and Pigments, Nano Energy, Computational & Theoretical Chemistry.*

SPOKEN LANGUAGES

1) Italian (native), 2) English (fluent), 3) Spanish (fluent), 4) Japanese (good: katakana, hiragana, about 1000 kanjis), 5) French (basic), 6) German (basic)

COMPUTATIONAL SKILLS

-OS: UNIX & LINUX systems; DOS and WINDOWS;
-Programming languages: FORTRAN, C, C++
-Computational Programs: Gaussian, ADF GAMESS-UK, SIESTA, PWscf, VASP, GULP, Yambo, Bader

MEMBERSHIPS & AFFILIATIONS

Materials Research Society (MRS)

RESEARCH INTERESTS

Density Functional Theory (DFT); Post-DFT methodologies (GW, Bethe-Salpeter Equation); Solid State Physics; Optical Properties of Materials with Applicability in Photocatalysis and Photovoltaics; Excitons and Quasi-Particles; Organic-Inorganic Semiconductors; Nanotechnology.
Computational chemical physics, bulk properties, surface science, and nanotechnology of:

1) *Hybrid Organic Inorganic Halide Perovskites*
2) *Semiconductor Nanostructured Materials* (nanosheets, nanorods, nanoclusters, etc…)
3) *Fully Inorganic Perovskite: Oxynitrides and Halides*.
4) *Carbonaceous layers for H_2 storing/molecular filtering (graphene, graph-N-yne)*

RESEARCH EXPERIENCE

- Modelling semiconductor surfaces/interfaces
  - Silicon technological surfaces and interfaces with high-*k* oxides (*ab-initio*)
  - Transport properties along Si/ZrO_2 and Si/HfO_2 interfaces (*ab-initio*)
  - Optical properties (excitons) of TiO_2 surfaces and nanosheets (*ab-initio*, MBPT, BSE) for photocatalytic applications.
  - Molecular anchoring on TiO_2 amorphous and surfaces (*ab-initio*)
  - Optical/structural properties graphene/TiO_2 nanocomposites (*ab-initio*)
- Modelling of IV-III/V alloys
  - Optical properties of Ge-doped GaAs (ab initio, QS*GW*).

PROJECTS, FUNDS, GRANTS (RECENT ACTIVITY)

2017 FFABR: *Fondo per il finanziamento delle attività base di ricerca.*
Grant by MIUR (3000 euros. Funded, P.I.)

2017−2018 ISCRA Project: IsC54
AccountID: CLUSper
OriginID: HP10CN7DI0
Science Domain: Condensed Matter Physics
Validity: Wed, 9 August, 2017 to Wed, 9 May, 2018
(Principal Investigator, P.I.)

2016−2017 ISCRA Project: IsC43 GAPBI
OriginID: HP10C79G0F
Science Domain: Condensed Matter Physics
Validity: Thursday, 21 July, 2016 to Friday, 21 April, 2017 (P.I.)

2016−2017 PRACE Proposal n°2016153664
UNWRAP: UNderstanding Water induced degRAdation of hybrid Perovskites (Collaborator).

2013−2015 Member of the CREST project "Phase Interface Science for Highly Efficient Energy Utilization" Theoretical design of photo-induced phase-interface elementary processes based on computational energy conversion science.
(Research Director: Prof. Koichi Yamashita).

2012-2013 ISCRA Project: IsC09 HyONaPh
OriginID: HP10CGTXSL HyONaPh
Science Domain: Condensed Matter Physics
Validity: Tuesday, 2 October, 2012 to Wednesday, 2 October, 2013
(Collaborator)

2012−2013 Member of the "Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST Program)": ⑤理論計算化学によ る有機系太陽電池の基礎科学 Theoretical analysis and optimization of TiO_2/dyes interfaces with applicability in DSSC.

2012 ETSF project (Out ref.: 433) titled "Non-isovalent alloys for photocatalysis & photovoltaics", in collaboration with the University of Rome, Tor Vergata. (P.I.)

2011-2013 ISCRA Project: IsC07 MagMang
OriginID: HP10C5WNRN MagMang
Science Domain: Computational Chemistry
Validity: Monday, 19 December, 2011 to Tuesday, 19 February, 2013
(Collaborator)

2011-2013 ISCRA Project: IsB04 ExNATiO
OriginID: HP10BUJ6VJ ExNATiO
Science Domain: Condensed Matter Physics
Validity: Thursday, 15 December, 2011 to Monday, 15 April, 2013
(Collaborator)

2011-2012 ISCRA Project: Project: IsB03 ZincOGaN
OriginID: HP10BJ1XJM ZincOGaN
Science Domain: Condensed Matter Physics
Validity: Thursday, 19 May, 2011 to Friday, 19 October, 2012
(Collaborator)

2010 ETSF (European Theoretical Spectroscopy Facility) project (Out ref.: 309) titled "A combined structural, electronic, and optical analysis of low dimensional titania based systems", in collaboration with the University of Rome Tor Vergata. (P.I.).

2007 PRIN 2007 Indagini teoriche accurate di sistemi di interesse per i processi atmosferici. ("Accurate theoretical investigations on systems of interest in atmospheric processes") Coordinator: Prof. G. De Petris, Person in charge: Prof. A. Sgamellotti (duration 24 months. Role: participant). (funded).

2005 PRIN 2005 Studio e caratterizzazione teorica di specie chimiche di interesse nei processi atmosferici. ("Theoretical Study and Charcterization of Chemical Species of interest in atmospheric processes.) Coordinator: Prof. G. De Petris, Person in charge: Prof. A. Sgamellotti (duration 24 months. Role: participant). (funded).

2004 HPC-Europa grant for a project on The Mechanism of Magnetic Interaction in Spin-Ladder Molecular Magnets, Department of Physical Chemistry, University of Barcelona (UB)/CESCA-CEPBA, Barcelona, Spain. (duration 2 months: Role: P. I.). (funded)

PUBLICATIONS

(**J**: journal; **B**=Book Chapter; **C**=Conference Abstract; **CP**=Procedure)

As Editor

-**Guest Editor** for *Taylor & Francis/CRC Book* of the Volume "*Theoretical Modeling of Organohalide Perovskites for Photovoltaic Applications*" (Jul 27th 2017)

Identifiers: LCCN 2016058861| ISBN 9781498750783 (hardback; alk. paper) | ISBN 1498750788 (hardback; alk. paper) | ISBN 9781498750790 (e-book) | ISBN 1498750796 (e-book)

-**Guest Associate Editor** "Materials Design and Optimization for Next Generation Solar Cell and Light-Emitting Technologies" Research Topic in Frontiers in Energy Research, Solar Energy (https://www.frontiersin.org/research-topics/7725/materials-design-and-optimization-for-next-generation-solar-cell-and-light-emitting-technologies)

-**Section Editor** "Current Opinion in Green and Sustainable Chemistry" (Elsevier). Section "Novel Materials for Energy Production and Storage".

Editorial: "A route for minimizing emissions: sun-mediated processes & clean batteries"

As Author

SCIENTIFIC JOURNALS

2019

J66. **G. Giorgi**

"Structural and electronic features of Si/$CH_3NH_3PbI_3$ interfaces with optoelectronic applicability: Insights from first-principles", *Nano Energy* (2019), doi.org/10.1016/j.nanoen.2019.104166

J65. Q. Zhang, S. Huang, J. Deng, D. Thrithamarassery Gangadharan, F. Yang, Z. Xu, **G. Giorgi**, M. Palummo, M. Chaker, D. Ma,

"Ice-Assisted Synthesis of Black Phosphorus Nanosheets as a Metal-Free Photocatalyst: 2D/2D Heterostructure for Broadband H_2 Evolution", *Adv. Funct. Mater.* (2019), 1902486.

J64. S. Manzhos, A. Pal, Y. Chen, **G. Giorgi,**

"Effect of Organic Cation States on Electronic Properties of Mixed Organic-Inorganic Halide Perovskite Clusters", *Phys. Chem. Chem. Phys*., (2019), 21, 8161-8169.

J63. L. Valentini, S. Bittolo Bon, M. Hernández, M.A. Lopez-Manchado, **G. Giorgi,**

"Synergistic icephobic behaviour of swollen nitrile butadiene rubber graphene and/or carbon nanotube composites", *Composites Part B: Engineering,* 166 (2019), 352-360

2018

J62. G. Giorgi, K. Yamashita, M. Palummo,

"Nature of the Electronic and Optical Excitations of Ruddlesden-Popper Hybrid Organic-Inorganic Perovskites: the Role of the Many-Body Interactions", *J. Phys. Chem. Lett.,* 9 (2018), 5891–5896

J61. G. Giorgi, K. Yamashita, M. Palummo,

"Two-dimensional optical excitations in mixed–valence $Cs_2Au_2I_6$ fully inorganic double perovskite"

J. Mater. Chem. C, 6 (2018) 10197-10201.

J60. G. Giorgi, K. Yamashita, H. Segawa,

"First-Principles Investigation of the Lewis Acid-Base Adduct Formation at the Methylammonium Lead Iodide Surface", *Phys. Chem. Chem. Phys*. 20 (2018) 11183-11195.

2017

J59. A. Kubo, **G. Giorgi**, K. Yamashita

"$MgTaO_2N$ Photocatalysts: Perovskite versus Ilmenite Structure. A Theoretical Investigation"

J. Phys. Chem. C, 121 (2017) 27813-27821

J58. D. Varsano, **G. Giorgi**, K. Yamashita, M. Palummo

"Role of Quantum-Confinement in Anatase Nanosheets", *J. Phys. Chem. Lett*., 8 (2017) 3867–3873

J57. J.-i. Fujisawa, T. Eda, **G. Giorgi**, M. Hanaya

"Visible-to-Near-IR Wide-Range Light Harvesting by Interfacial Charge-Transfer Transitions between TiO_2 and *p*-Aminophenol and Evidence of Direct Electron Injection to the Conduction Band of TiO_2", *J. Phys. Chem. C*, 121 (2017) 18710–18716

J56. T. Hata, **G. Giorgi**, K. Yamashita, C. Caddeo, A. Mattoni,

"Development of a Classical Interatomic Potential for $MAPbBr_3$", *J. Phys. Chem. C*, 121 (2017) 3724–3733

2016

J55. A. Kubo, **G. Giorgi**, K. Yamashita,

"Anion Ordering in $CaTaO_2N$: Structural Impact on the Photocatalytic Activity. Insights from First-Principles", *Chem. Mater.*, 29 (2017) 539–545

J54. M. Bartolomei, **G. Giorgi**,

"A Novel Nanoporous Graphite Based on Graphynes: First-Principles Structure and Carbon Dioxide Preferential Physisorption", *ACS Appl. Mater. Interfaces*, 8 (2016), 27996–28003.

J53. G. Giorgi, T. Yoshihara, K. Yamashita,

"Structural and electronic features of small hybrid organic-inorganic halide perovskite clusters: a theoretical analysis", *Phys. Chem. Chem. Phys.*, 18 (2016) 27124 - 27132, Invited paper for the "Physical chemistry of hybrid perovskite solar cells" issue.

J52. T. Hata, **G. Giorgi**, K. Yamashita,

"The Effects of the Organic–Inorganic Interactions on the Thermal Transport Properties of $CH_3NH_3PbI_3$" *Nano Lett.*, 16 (2016) 2749–2753.

J51. G. Giorgi, K. Yamashita,

"Zero-Dimensional Hybrid Organic–Inorganic Halide Perovskite Modeling: Insights from First Principles", *J. Phys. Chem. Lett.*, 7 (2016) 888–899. *Perspective article*.

J50. T. Asami, **G. Giorgi**, K. Yamashita, P. Belanzoni.

"Study on the Phenomenon Reported "Neutron Generation at Room Temperature in a Cylinder Packed with Titanium Shavings and Pressurized Deuterium Gas" (3)." JOURNAL OF CONDENSED MATTER NUCLEAR SCIENCE, 18, (2016) 24-35.

2015

J49. G. Giorgi, K. Yamashita,

"Zero-dipole molecular organic cations in mixed organic–inorganic halide perovskites: possible chemical solution for the reported anomalous hysteresis in the current–voltage curve measurements", *Nanotechnology*, 26 (2015) 442001-16. (*Invited Topical Review Article* to 'Perovskite Solar Cells', Sum & Park Editors, themed issue paper,)

J48. G. Giorgi, K. Yamashita,
"Organic-Inorganic halide perovskites: an ambipolar class of materials with enhanced photovoltaic performances", *J. Mater. Chem. A* 3 (2015) 8981 – 8991.
(*Invited Review Article* to 'Perovskite Solar Cells', Lin, Park, and Li Editors, themed issue paper).

J47. M. Bartolomei, E. Carmona-Novillo, **G. Giorgi,**

"First Principles Investigation of Hydrogen Physical Adsorption on Graphynes' layers",

Carbon, 95 (2015) 1076–1081.

J46. G. Giorgi, K. Yamashita,
"Alternative, lead-free, hybrid organic-inorganic perovskites for solar applications: a DFT analysis", *Chem Lett.* 44 (2015) 826-828.

J45. G. Giorgi, J.-I. Fujisawa, H. Segawa, K. Yamashita,

"Organic-Inorganic Hybrid Lead-Iodide Perovskite Featuring Zero-Dipole-Moment Guanidinium Cations: A Theoretical Analysis" *J. Phys Chem C,* 119 (2015) 4694–4701. (*Editor's Choice*).

J44. H. Kawai, **G. Giorgi**, A. Marini, K. Yamashita,

"The mechanism of slow hot-hole cooling in lead-iodide perovskite: First-principle calculations on electron-phonon carrier lifetimes" *Nano Lett.*, 15 (2015) 3103–3108.

J43. S. Manzhos, **G. Giorgi**, K. Yamashita,

"A Density Functional Tight Binding Study of Acetic Acid Adsorption on Crystalline and Amorphous Surfaces of Titania" *Molecules*, **(**2015) 20, 3371-3388.

2014

J42. M. Bartolomei, E. Carmona-Novillo, M. Hernández, J. Campos-Martínez, F. Pirani, **G. Giorgi,**

"Graphdiyne Pores: 'Ad Hoc' Openings for Helium Separation Applications", *J. Phys. Chem. C*, 118 (2014) 29966-29972.

J41. X.-F. Yu, **G. Giorgi**, H. Ushiyama, K. Yamashita,

"First principle study of fast diffusion in Na_3P", Chem. Phys. Lett. 612 (2014) 129–133.

J40. G. Giorgi, J.-I. Fujisawa, H. Segawa, K. Yamashita,

"Cation Role in Structural and Electronic Properties of 3D Organic-inorganic Perovskite Halides: A DFT Analysis", *J. Phys. Chem. C*, 118 (2014) 12176–12183.

J39. Y. Masuda, **G. Giorgi,** K. Yamashita

"DFT study of anatase derived TiO_2 nanosheets/graphene hybrid materials"
Phys. Status Solidi B, 251 (2014) 1471–1479. *Editor's choice & Issue back coverpage*.

J38. J.-I. Fujisawa, **G. Giorgi**,

"Lead-iodide nanowire perovskite with methylviologen showing interfacial charge- transfer absorption: a DFT analysis", *Phys. Chem. Chem. Phys.,* 16 (2014) 17955-17959.

J37. M. Bartolomei, E. Carmona-Novillo, M. Hernández, J. Campos-Martínez, F. Pirani, **G. Giorgi,** K. Yamashita,
"The Penetration Barrier of Water through Graphynes' Pores: First-Principles Predictions and Force Field Optimization" *J. Phys. Chem. Lett.*, 5 (2014) 751–755

2013

J36. G. Giorgi, J.-I. Fujisawa, H. Segawa, K. Yamashita,

"Small Photocarrier Effective Masses Featuring Ambipolar Transport in Methylammonium Lead-Iodide Perovskite: A Density Functional Analysis", *J. Phys. Chem. Lett.*, 4 (2013) 4213–4216.

J35. G. Giorgi, P. Belanzoni, T. Asami, K. Yamashita

"On the dual deuterium/deuteron nature of D charge distribution in the Ti host matrix: A DFT analysis", *Int. J. Hydrogen Energy*, 38 (2013) 16477-16484.

J34. S. Manzhos, **G. Giorgi**

"Bridging the Fields of Solar Cell and Battery Research to Develop High- Performance Anodes for Photoelectrochemical Cells and Metal Ion Batteries" *Challenges*, 4 (2013) 116-135.

J33. J.-W. Song, **G. Giorgi**, K. Yamashita, K. Hirao

"Singularity-free hybrid functional with a Gaussian-attenuating exact exchange in a plane-wave basis", *J. Chem. Phys.*, 138, (2013) 241101.

J32. G. Giorgi, J.I. Fujisawa, H. Segawa, K. Yamashita

"Unravelling Adsorption Mechanism of Aromatic and Aliphatic Diols on TiO_2 Surface by Density Functional Theory Analysis", *Phys. Chem. Chem. Phys.,* 15 (2013) 9761-7.

2012

J31. G. Giorgi, P. Belanzoni, T. Asami, K. Yamashita,

"Neutron generation via the mechanism adsorption of pressurized deuterium on an electron deficient titanium matrix. An MD–DFT combined analysis on the mechanism of the Ti–D bond formation", *Int. J. Hydrogen Energy*, 37 (2012) 18959.

J30. M. Palummo, **G. Giorgi**, L. Chiodo, A. Rubio, K. Yamashita,

"The nature of radiative transitions in TiO_2-based nanosheets", *J. Phys. Chem. C*, 116 (2012) 18495

J29. H. Kawai, **G. Giorgi**, K. Yamashita,

"Impact of short-range order and clustering effect on the bandgap bowing: first-principles calculations on the electronic properties of metastable $(GaAs)_{1-x}(Ge_2)_x$ alloys", *Phys. Status Solidi B,* 249 (2012) 29. Issue back coverpage.

2011

J28. G. Giorgi, M. Palummo, L. Chiodo, K. Yamashita,

"Excitons at the (001) surface of anatase: Spatial behavior and optical signatures", *Phys. Rev. B,* 84, (2011) 073404.

J27. H. Kawai, **G. Giorgi**, K. Yamashita,

"Clustering and Octet Rule Violation Impact on Band Gap Bowing: Ab Initio Calculation of the Electronic Properties of $(GaAs)_{1-x}(Ge_2)_x$ Alloys", *Chem. Lett.*, 40 (2011) 770.

J26. G. Giorgi, K. Yamashita,

"Amphoteric behaviour of Ge in GaAs: an LDA+*U* analysis", *Modelling Simul. Mater. Sci. Eng.***,** 19 (2011) 035001.

J25. G. Giorgi, K. Yamashita,

"Stress analysis of silicon nanosheets with nanotechnological functionalization",
in Special Issue on "Nano-Engineered Silicon: Technology and Applications", *Sci. Adv. Mater.,* 3 (2011) 455.

J24. P. Belanzoni, **G. Giorgi**, K. Yamashita,

"Functionalization of atomically flat, hydrogen terminated, (1×1) and (2×1)-(1 0 0) silicon surfaces via reaction with 1-alkyne: a DFT study",
in Special Issue on "Nano- Engineered Silicon: Technology and Applications", *Sci. Adv. Mater.,* 3 (2011) 436.

J23. A. Orbelli Biroli, F. Tessore, M. Pizzotti, C. Biaggi, R. Ugo, S. Caramori, C. Bignozzi, F. De Angelis, **G. Giorgi**, E. Licandro,
"A Multitechnique Physicochemical Investigation of Various Factors Controlling the Photoaction Spectra and of Some Aspects of the Electron Transfer for a Series of Push–Pull Zn(II) Porphyrins Acting as Dyes in DSSCs", *J. Phys. Chem. C*, 115 (2011) 23170.

2010

J22. G. Giorgi, M.Van Schilfgaarde, A. Korkin, K. Yamashita,

"On the chemical origin of the gap bowing in $(GaAs)_{1-x}$ Ge_{2x} alloys: a combined DFT- QSGW study", *Nanoscale Res. Lett.*, 5 (2010) 469.

J21. G.F. Cerofolini, E. Romano, D. Narducci, P. Belanzoni and **G. Giorgi**
"Assigning chemical configurations to the XPS features observed at pristine (1 0 0) Si surface resulting after etching in HF aqueous solution", *Appl. Surf. Sci.,* 256 (2010) 6330.

2009

J20. P. Belanzoni, **G. Giorgi**, A. Sgamellotti, and G. F. Cerofolini
"Silylene Defect at the Dihydrogen Terminated (100) Si Surface", *J. Phys. Chem. A.* 113 (2009) 14375-14388.

J19. G.F. Cerofolini, E. Romano, **G. Giorgi**, and P. Belanzoni,

"Counterintuitive assignment of the lines observed by x-ray photoelectron spectroscopy at the hydrogen-terminated (1 0 0) surface of silicon", *J. Phys. D: Appl. Phys.*, 42 225301 (2009).

J18. G. Giorgi, L.R.C. Fonseca, A. Korkin, K. Yamashita,

"Impact of the crystal structure of HfO_2 on the transport properties of model HfO_2/Si/HfO_2 silicon-on-insulator field effect transistors: a combined DFT-scattering theory approach", *Phys. Rev. B,* 79, 235208 (2009)

J17. G.F. Cerofolini, **G. Giorgi***,* A. Sgamellotti, P. Belanzoni,

"How silylene defects at (100) Si surfaces can account for the anomalous features observed via x-ray photoelectron spectroscopy", *J. Chem. Phys.,* 130, 184702 (2009).

2008

J16. G. Giorgi, X. Cartoixà, A. Sgamellotti, R. Rurali

"Mn-doped silicon nanowires: First-principles calculations", *Phys. Rev. B,* (2008) 78, 115327.

J15. G. Giorgi, A. Korkin, K. Yamashita

"Zirconium and Hafnium Oxide Interface with Silicon: Computational Study of Stress and Strain Effects", *Comp. Mat. Sci.*, (2008) 43, 930-937.

2006

J14. C. Coletti, A. Marrone, **G. Giorgi**, A. Sgamellotti, G.F. Cerofolini, N. Re.

"Nonradical Mechanisms for the Uncatalyzed Thermal Functionalization of Silicon Surfaces by Alkenes and Alkynes: A Density Functional Study", *Langmuir*, (2006), 22, 9949-9956.

J13. P. Belanzoni, **G. Giorgi**, G.F. Cerofolini, A. Sgamellotti.

"The silicon carbonyls revisited: on the existence of a planar $Si(CO)_4$", *Theor. Chem. Acc.*, (2006), 115, 448-459.

J12. P. Belanzoni, **G. Giorgi**, G.F. Cerofolini, A. Sgamellotti.

"Planar tetracoordinated silicon in silicon carbonyl complexes: a DFT approach", *J. Phys. Chem. A*, (2006) 110, 4582-4591.

J11. P. Belanzoni, **G. Giorgi**, G.F. Cerofolini.

"Reactivity of silicon carbonyl with ethylene", Chem. Phys. Lett., 418 (2006) 383-385.

2005

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"The Mechanism of Magnetic Interaction in Spin-Ladder Molecular Magnets: A First- Principles, Bottom-Up, Theoretical Study of the Magnetism in the Two-Legged Spin- Ladder Bis(2-amino-5-nitropyridinium) Tetrabromocuprate Monohydrate", *Eur. J. Inorg. Chem.,* (2005) 4697-4706. Issue Coverpage.

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J4. P. Belanzoni, **G. Giorgi**, G.F. Cerofolini

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J3. G. Giorgi, F. De Angelis, N. Re, A. Sgamellotti

"A theoretical investigation of the Chalk-Harrod and modified Chalk-Harrod mechanisms involved in hybrid integrated circuit building."
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BOOK CHAPTERS

B4. J. Even, **G. Giorgi**, C. Katan, H. Kawai, and K. Yamashita,

"Organic–Inorganic Halide Perovskite Quasi-Particle Nature Analysis via the Interplay among Classic Solid-State Concepts, Density Functional, and Many-Body Perturbation Theory".
CRC Press Books - "Theoretical Modeling of Organohalide Perovskites for Photovoltaic Applications", (**Giacomo Giorgi** & Koichi Yamashita Editors)
CRC Press Taylor & Francis Group, Boca Raton 2017, pages 201-223.

B3. L. Chiodo, **G. Giorgi**, M. Palummo,

"Electronic and Optical Properties of Oxides Nanostructures by First-Principles Approaches". (Bharat Bhushan Editor).
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B2. G. Giorgi, K. Yamashita,

"Electronic and Optical Properties of Low-Dimensional TiO2: From Minority Surfaces to Nanocomposites".
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B1. G. Giorgi, H. Kawai, K. Yamashita,

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PEER REVIEWED CONFERENCE ABSTRACTS

C17. G. Giorgi,

"Hybrid Organic-Inorganic Halide Perovskites: Dimensionality vs. Applicability. A Theoretical Standpoint."

Nano and Giga Challenges in Electronics, Photonics and Renewable Energy, Symposium and Summer School (Tutorial Lectures), Tomsk, Russia, Sept. 18-22, 2017

C16. M. Kaneko, **G. Giorgi**, K. Yamashita,

"Photoexcitation Mechanism of Metallic $Sr_{1-x}NbO_3$ for Watersplitting Photocatalyst" - **Bulletin of the American Physical Society**, 2017. APS March Meeting 2017, Vol. 62, 4; Mar 13–17, 2017; New Orleans, Louisiana, USA

C15. T. Hata, **G. Giorgi**, K. Yamashita,

"Origin of low thermal conductivity in organic-inorganic thermoelectric materials" - **Bulletin of the American Physical Society**, 2017. APS March Meeting 2017, Vol. 62, 4; Mar 13–17, 2017; New Orleans, Louisiana, USA

C14. G. Giorgi, K. Yamashita

"Zero-Dimensional Hybrid Organic–Inorganic Halide Perovskite Modeling: Insights from First Principles", Vth Spanish-Portuguese Workshop on Photochemistry, Facultad de Ciencias Ambientales y Bioquímica, e INAMOL "Campus Tecnológico, Fábrica de Armas", University of Castilla-La Mancha (UCLM), September 7-10, 2016 | Toledo, Spain.

C13. G. Giorgi, K. Yamashita

"Hybrid Organic-Inorganic Halide Perovskites Nanoclusters: Insights from First Principles Calculations", 2016 **MRS Spring Meeting & Exhibit**. Mar 28th–Apr 1st, 2016. Phoenix, Arizona (USA).

C12. **G. Giorgi**, J. I. Fujisawa, H. Segawa, K. Yamashita

"Organic-inorganic hybrid lead iodide perovskite with zero-dipole-moment guanidinium ($GA=C(NH_2)_3^+$) cations: a Density Functional based analysis", **Bulletin of American Physical Society**, APS March Meeting 2015, San Antonio, TX, (USA). March 2-6th.

C11. **G. Giorgi**, J. I. Fujisawa, H. Segawa, K. Yamashita

"The Ambipolar Nature of Mixed Organic-Inorganic Halide Perovskites: A DFT Investigation", **2014 MRS Fall Meeting & Exhibit,** 2014 Boston, Massachusetts (USA). Nov 29th – Dec 5th

C10. G. Giorgi, J.-I. Fujisawa, H. Segawa, K. Yamashita

"'The role of the methylammonium cation in the structural and electronic properties of 3D organic-inorganic perovskite halides: a DFT analysis including Spin Orbit Coupling", **Bulletin of the American Physical Society**, APS March Meeting 2014, Denver, CO (USA). 2014 Mar 3-7th.

C9. G. Giorgi, J.-I. Fujisawa, H. Segawa, K. Yamashita

"The role of the organic cation MA ($CH_3NH_3^+$) in pseudocubic 3D $MAPbI_3$ organic-inorganic perovskites", **Nano and Giga Challenges in Electronics, Photonics and Renewable Energy. From Materials to Devices to System Architecture Symposium and Spring School**. Phoenix, Arizona (USA) Mar 10-14th, 2014.

C8. G. Giorgi, M. Palummo, A. Rubio, K. Yamashita

"Radiative transitions and optical signatures in TiO_2 minority surfaces and their derived nanosheets", **Nano and Giga Challenges in Electronics, Photonics and Renewable Energy. From Materials to Devices to System Architecture Symposium and Spring School**. Phoenix, Arizona (USA) Mar 10-14th, 2014.

C7. H. Kawai, **G. Giorgi**, M. Palummo, K. Yamashita

"The first-principles study on the electronic and optical properties of $(Ga_{1-x}Zn_x)(N_{1-x}O_x)$ from many-body perturbation theory", **Bulletin of the American Physical Society**, APS March Meeting 2013, Baltimore (USA).

C6. Y. Masuda, **G. Giorgi**, K. Yamashita

"Theoretical study on electronic properties of 2D graphene-TiO_2 nanocomposites" **Bulletin of the American Physical Society**, APS March Meeting 2013, Baltimore (USA).

C5. **G. Giorgi**, M. Palummo, L. Chiodo, A. Rubio, K. Yamashita

"The Nature of Radiative Transitions in TiO2-based Nanosheets"

2012 MRS Fall Meeting & Exhibit, Nov 25-30th, 2012 Boston, Massachusetts (USA).

C4. G. Giorgi, M. Van Schilfgaarde, A. Korkin, K. Yamashita,

"Chemical origin of the gap bowing in $(GaAs)_{1-x}Ge_{2x}$ alloys: A combined DFT–QSGW study", **Materials & Nanotechnology Computational Chemistry in Materials and Nanotechnology** (#182) – **6th ACS Pacifichem** 2010 Hawaii, USA

C3. G. Giorgi, L.R.C.Fonseca, A. Korkin, K. Yamashita

"A combined DFT-scattering theory approach for transport properties calculation of HfO_2/Si/HfO_2 silicon-on-insulator FET" **Nano and Giga Challenges in Electronics,Photonics and Renewable Energy & 14th Canadian Semiconductor Technology Conference,** Hamilton, Ontario, Canada, Aug 10-14th, 2009

C2. G. Giorgi, A. Korkin, K. Yamashita

"ZrO_2 and HfO_2 Interface with Silicon: a DFT Study of Stress and Strain Effects" **213th ECS Meeting, Phoenix AZ, USA. Meet. Abstr. - Electrochem. Soc**.(2008) 801, 655

C1. G. Giorgi, P. Belanzoni, G. Cerofolini, A. Sgamellotti

"Theoretical investigations on atomic-silicon cryptates in siloxanic networks", **Nano and Giga Challenges in Microelectronics Symposium and Summer School Research and Development Opportunities**, Cracow, Poland, Sep 13-17th, 2004.

CONFERENCE PROCEEDINGS

CP4. G. Giorgi, M. Palummo, L. Chiodo, A. Rubio, J.-I. Fujisawa, H. Segawa and K. Yamashita

"**Minority surfaces of anatase and their derived nanosheets: a combined DFT and MBPT analysis**" Nanoenergy 2013, International Conference – Perugia, ITALY, July 10-13, 2013 – NANOENERGY LETTERS n. 6 - August 1,. Perugia, ITALY, 2013, pag. 49-50, no doi provided (*http://www.nanoenergyletters.com/node/189*)

CP3. P. Belanzoni, **G. Giorgi**, G.F. Cerofolini

"**Bonding Configurations and Observed XPS Features at the Hydrogen Terminated (100) Si Surface: What Can We Gain from Computational Chemistry**", LNCS Volume 7971.

13th International Conference on Computational Science and Its Applications (ICCSA2013) Ho Chi Minh City, Vietnam, June 2013 Proceedings, Part I,

Editors: B. Murgante, S. Misra, M. Carlini, C. M. Torre, H.-Q. Nguyen, D. Taniar, B. O. Apduhan, O. Gervasi, Springer Berlin Heidelberg, 2013, pp 57-68 ISBN: 978-3-642-39636-6 (Print) 978-3-642-39637-3 (Online).

CP2. **G. Giorgi**, F. De Angelis, N. Re, A. Sgamellotti

"**Theoretical Analysis on Mechanisms Implied in Hybrid Integrated Circuit Building**",

LNCS, Vol. 2658, Computational Science — ICCS 2003, International Conference Melbourne, Australia and St. Petersburg, Russia June 2–4, 2003 Proceedings, Part II, Editors: P. M. A. Sloot, D. Abramson, A. V. Bogdanov, Y. E. Gorbachev, J. J. Dongarra, A. Y. Zomaya, Springer Berlin Heidelberg 2003, pp. 331-340. ISBN: 978-3-540-40195-7 (Print) 978-3-540-44862-4 (Online).

CP1. **G. Giorgi**, K. Yamashita*

"**Electronic and Optical Properties of Nitrogen-Doped Layered Manganese Oxides**"

"Ceramics for Environmental and Energy Applications II: Ceramic Transactions Vol 246", 10th Rim Conference on Ceramic and Glass Technology, Coronado, California. Jun 2-6, 2013.

Editors: F. Dogan, T. M. Tritt, T. Sekino, Y. Katoh, A. J. Pyzik, I. Belharouak, A. R. Boccaccini, J. Marra. Volume Editor: H.-T. Lin

The American Ceramic Society, John Wiley & Sons, Inc. Hoboken, New Jersey (2014) 135-140. ISBN: 978-1-118—77124-2. ISSN: 1042-1122.

INVITED SEMINARS

13) "Excitons, Phonons, and Electron-Phonon coupling in 3D and in Mixed 3D/2D Hybrid Perovskites",

2019, Feb 12th, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan

12) "Perovskites in sun-to-energy conversion. Insights from first-principles",

2019, 23rd Jan. Department of Chemistry and Biochemistry, The University of Bern, Switzerland.

11) "Hybrid Materials for Solar-to-Energy conversion: a theoretical standpoint".

2018, 10th Sept, XIII-EM-TCCM, European Master in Theoretical Chemistry and Computational Modelling,13th International Intensive Course, Dipartimento di Matematica e Informatica, University of Perugia, Italy.

10) "Low-dimensional Systems for Optoelectronics and Self-cleaning Applications"

2018, 10th Sept, XIII-EM-TCCM, European Master in Theoretical Chemistry and Computational Modelling,13th International Intensive Course, Dipartimento di Matematica e Informatica, University of Perugia, Italy

9) "Hybrid Organic-Inorganic Halide Perovskites: a novel class of Materials for the renaissance of renewables. A theoretical standpoint", 2017 13st Oct, Department of Chemistry, Università di Tor Vergata, Rome, Italy.

8)"Hybrid Organic-Inorganic Halide Perovskites from 3D to 0D: Insights from First Principles Calculations", 2017 31st Mar, ICMAB - Sala d'actes Carles Miravitlles. UAB, Barcelona, Spain.

7) Special Lecture "Theoretical Chemistry for Next-generation Photovoltaics.

→7a. Organic-Inorganic halide perovskites. From 3D to 0D: experiments meet theory.

→7b. Alternative cations in organic-inorganic halide perovskite: a playground for enhancing performances and solving environmental issues.

→7c. Non-graphenic layered carbonaceous materials: from hydrogen storing to photovoltaics.

→7d. Structural, electronic, and excitonic properties of nanostructured TiO_2 derived materials.

→7e. Surface on surface and molecule on surface: Interfaces *vs*. molecular adsorption. Insights from first-principles.

Jan 30th 2017Place: Bld.#15 Room 101, Komaba Campus, The University of Tokyo. Tokyo, JAPAN.

6) "Hybrid Organic-Inorganic Halide Perovskites: Ambipolar Materials for Solar-to Energy Conversion", Jan 20th 2017, Ciriaf, The University of Perugia, ITALY.
(Class for the doctoral course "Dottorato di Ricerca in Energia e Sviluppo Sostenibile", XXXII ciclo A.A. 2016 - 2017)

5) "Brief introduction to the VASP code. Theory and examples".Nov 19th 2015, Institute for Chemical Research (Prof. Wakamiya's group), Kyoto University, JAPAN.

4) "From hybrid perovskites to TiO_2/graphene nanohybrids. Performing materials in PV and photocatalysis". Dec 22nd 2014, Computational Laboratory for Hybrid and Organic Photovoltaics, Institute of Molecular Sciences and Technologies (CNR-ISTM), c/o Department of Chemistry, The University of Perugia, ITALY.

3) "DFT study on organic-inorganic perovskites: the role of methylammonium cation" May 8th 2014, Advanced Institute of Science & Technology (AIST), Tsukuba, JAPAN.

2) "The nature of radiative transitions in TiO_2-based nanosheets" May 15th, 2012, Yokohama National University, Yokohama, JAPAN.

1) "Optical properties of device oriented materials. Alloys, surfaces, & nanosheets, through Density Functional and Many Body Perturbation Theory"
"Materials modelling – Hierarchies on the Atomic Scale",
Apr 16-17th, 2012, RWTH, Institut fur Gesteinshuettenkunde, Aachen , GERMANY.

CONFERENCE CONTRIBUTIONS

-INVITED TALKS

15) "Excitons in Ruddlesden-Popper Hybrid Organic-Inorganic Perovskites: Optical Signatures and Spatial Localization" in

"International workshop on evaluation method for perovskite solar cells",

Kyoto, JAPAN, Jan 30th 2019

14) "Excitons in 3D Pb-free Bulk and in Mixed 3D/2D Hybrid Perovskites" in

"IRSEC18, 6th International Renewable and Sustainable Energy Conference",

Rabat, MOROCCO, Dec 6th 2018 (*Keynote Speaker*).

13) "Ab-initio study of electronic & optical properties of organic-inorganic 2D and 2D/3D perovskites: the role of many-body effects" in

"Electronic and Structural Dynamics in Hybrid Perovskites: Theory Meets Experiment", Telluride, CO, USA, Jul 17-21st, 2018.

12) "Hybrid Organic-Inorganic Halide Perovskites: Dimensionality vs. Applicability. A Theoretical Standpoint" in:

"Nano and Giga Challenges in Electronics, Photonics and Renewable Energy", Symposium and Summer School (Tutorial Lectures),

Tomsk, Russia, Sept. 18-22nd, 2017.

11) "Inorganic and Organic-Inorganic Perovskites for Solar-to-Energy Applications. A Theoretical Analysis" in:

"4th Workshop on Present Status and Future Perspective of Perovskite Solar Cells", Feb 6th, 2017, ENEOS Hall, RCAST, The University of Tokyo. Tokyo, Japan.

10) "Hybrid Organic-Inorganic Halide Perovskites Materials for Photovoltaics: Insights from First Principles" in:

"12th Workshop on the Future Direction of Photovoltaics",
Jan 28-29th, 2016, Tokyo Tech Front, Tokyo Institute of Technology. Tokyo, Japan.

9) "A Theoretical Study of the Perovskite Solar Cells" in:

"Workshop of the Electrochemical Society of Japan on perovskite solar cells".

Dec 3rd, 2015, RCAST, Komaba. The University of Tokyo, Japan.

8) "Hybrid Organic-Inorganic Perovskites: the Renaissance of a Unique Class of Materials. A Theoretical Point of View" in:

"Tokai conference 2015 in Nagano", Oct 10th, 2015, Shinshu University, Japan.

7) "The Quest of Performing Materials in Photocatalysis & Photovoltaics: New Tricks for Old Dogs" in:

"New Challenges for Sustainable Developments", Sept 7th 2015, The University of Perugia, Italy.

6) "Guandinium (GA=$^{+}C(NH_2)_3$) based hybrid organic-inorganic perovskites: a theoretical analysis" in:

"Cecam workshop: Perovskite solar cells: the quest for a theoretical description", Aug 25-28th 2015, CECAM-HQ-EPFL, Lausanne, Switzerland.

5) "Chemical solutions for the working and environmental issues in mixed organic-inorganic perovskites: a density functional based investigation" in:

"Energy Materials & Nanotechnology – EMN Qingdao Meeting". Jun 14-17th 2015, Qingdao, CHINA.

4) "Organic cation role in the $MAPbI_3$ ($MA=CH_3NH_3^+$) organic-inorganic halide perovskite" in:
"Energy Material Nanotechnology–EMN Summer Meeting".
Jun 9-12th 2014, Cancun, MEXICO.

3) "DFT study on organic-inorganic perovskites" in:
"FIRST International Open Symposium for Scientists: Organic Photovoltaics Tap Our Future". Feb 5th 2014, Ito hall, Hongo Campus, The University of Tokyo, JAPAN.

2) "Materials for Solar Energy Conversion: A Theoretical Study" in:
"FIRST International Symposium for Young Students; Challenge of Chemistry toward Solar Energy Utilization". Feb 8th 2014, ENEOS hall, Environmental Energy Research Building, (#3 Annex), Research Center for Advanced Science and Technology (RCAST), The University of Tokyo, JAPAN.

1) "Excitonic effect on TiO_2 (001) surfaces" in:

"Titania for all seasons: Multifunctionality of an undercover semiconductor",
Sep 06-10th 2010, Bremen Center for Computational Materials Science, Bremen, GERMANY

OTHER CONFERENCE CONTRIBUTIONS
(**O.P.**=Oral Presentation; **P.P.**=Poster Presentation)

44) G. Giorgi,

"Hybrid Organic-Inorganic Halide Perovskites for Photovoltaics and Lasing Applications: Insights from First Principles Calculations" **(O.P.)**
"XXXVI Biennial Meeting of the Real Sociedad Española de Física", Symposium (GEFAM) "MOLECULAR PHYSICS IN THE EDGE"
Santiago de Compostela, Spain, Jul 17-21, 2017.

43) M. Bartolomei, ***G. Giorgi***,

"Novel Nano-porous Graphites for Gas Storage and Release" **(P.P.)**
"XXXVI Biennial Meeting of the Real Sociedad Española de Física", Symposium (GEFAM) "MOLECULAR PHYSICS IN THE EDGE"
Santiago de Compostela, Spain, Jul 17-21, 2017.

42) A. Kubo, ***G. Giorgi***, K. Yamashita
"Structural and electronic features of perovskite-type photocatalysts: Insights from first-principles" **(P.P.)** "2017 International Conference on Artificial Photosynthesis"

Suzaku Campus, Ritsumeikan University, Kyoto, Japan, Mar 2-5, 2017.

(*Awarded as the best poster of the conference*).

41) M. Kaneko, ***G. Giorgi***, K. Yamashita
"Photoexcitation mechanism of metallic $Sr_{1-x}NbO_3$ for water splitting photocatalyst" **(P.P.)**

"2017 International Conference on Artificial Photosynthesis" Suzaku Campus, Ritsumeikan University, Kyoto, Japan, Mar 2-5, 2017.

40) G. Giorgi,
"Hybrid Organic-Inorganic Halide Perovskites from 3D to 0D: Insights from First Principles Calculations" (**O. P.**).

"2nd International Conference on Perovskite Solar Cells and Optoelectronics (PSCO-2016)", Palazzo Ducale Genova, Italy, 26-28 September 2016

39) G. Giorgi, K. Yamashita
"Chemical Solutions for the Working and Environmental Issues in Mixed Organic-Inorganic Perovskites: A Theoretical Analysis". (**O. P.**)
"Annual Meeting of Japan Society for Molecular Science", Tokyo Institute of Technology, 2015, Sep 16-19th Tokyo, Japan

38) H. Iriguchi, ***G. Giorgi***, K. Yamashita
"Theoretical Studies of Structural & Electronic Properties of Doped $BaTaO_2N$ Systems" (**P.P.**)
"Annual Meeting of Japan Society for Molecular Science", Tokyo Institute of Technology, 2015, Sep 16-19th Tokyo, Japan.

37) A. Kubo, ***G. Giorgi***, K. Yamashita
"*Ab-initio* investigations on the anion ordering and bandstructure of oxynitride photocatalyst $CaTaO_2N$" (**P.P.**)
"Annual Meeting of Japan Society for Molecular Science",Tokyo Institute of Technology, 2015, Sep 16-19th Tokyo, Japan.

36) T. Hata, ***G. Giorgi***, K. Yamashita
"Structure Dependence on thermal transport properties of organic inorganic perovskites" (**P.P.**)
"Annual Meeting of Japan Society for Molecular Science", Tokyo Institute of Technology, 2015, Sept 16-19th Tokyo, Japan

35) M. Kaneko, ***G. Giorgi***, K. Yamashita
"Effect of Sr vacancies on the bandstructure of $SrNbO_3$: A DFT analysis" (**P.P.**)

"Annual Meeting of Japan Society for Molecular Science", Tokyo Institute of Technology, 2015, Sep 16-19th Tokyo, Japan.

34) G. Giorgi, J. I. Fujisawa, H. Segawa, K. Yamashita

"Organic-inorganic hybrid lead iodide perovskite with zero-dipole-moment guanidinium ($GA=C(NH2)3^+$) cations: a Density Functional based analysis", (**O.P.)**
2015 American Physical Society (APS), March Meeting,
Mar 2-6th, 2015, San Antonio, TX, USA

33) G. Giorgi, J. I. Fujisawa, H. Segawa, K. Yamashita
"The Ambipolar Nature of Mixed Organic-Inorganic Halide Perovskites: A DFT Investigation", (**O.P.)**
"2014 MRS Fall Meeting & Exhibit",
Nov 29th –Dec 5th, 2014 Boston, Massachusetts (USA).

32) M. Bartolomei; E. Carmona-Novillo, M. I. Hernández, J. Campos-Martínez; F. Pirani, ***G. Giorgi***, K. Yamashita,
"Water through Graphynes' Pores: First-Principles Penetration Barrier and Force Field Optimization", (**P.P.)**
(*Awarded as the best poster of the conference*).
"NANOStruc2014, International Conference on Structural Nano Composites"
20-21 May 2014 Madrid, SPAIN

31) H. Kawai, ***G. Giorgi***, K. Yamashita
"First-principles study on the impact of local chemical bonding on band gap and band edge position of $(Ga_{1-x}Zn_x)(N_{1-x}O_x)$ solid solution", (**P.P.)**
(*Awarded as the best poster of the conference*).
"7th Tokyo Conference on Advanced Catalytic Science and Technology (TOCAT7)",
Jun 1-6th 2014, Kyoto, JAPAN.

30) G. Giorgi, J.-I. Fujisawa, H. Segawa, K. Yamashita,
"The role of the organic cation MA ($CH_3NH_3^+$) in pseudocubic 3D $MAPbI_3$ organic-inorganic perovskites", (**P.P.)**
(*Awarded as the best poster of the conference*).
"Nano & Giga Challenges in Electronics, Photonics and Renewable Energy, From Material to Devices to System Architecture", Symposium and Spring School,
Mar 10-14th, 2014, Arizona State University (ASU) Phoenix, AZ, USA.

29) G. Giorgi, M. Palummo, A. Rubio, K. Yamashita,
"Radiative transitions and optical signatures in TiO_2 minority surfaces and their derived nanosheets", (**O.P.)**
"Nano & Giga Challenges in Electronics, Photonics and Renewable Energy, From Material to Devices to System Architecture", Symposium and Spring School,
Mar 10-14th, 2014, Arizona State University (ASU) Phoenix, AZ, USA.

28) G. Giorgi, J.-I. Fujisawa, H. Segawa, K. Yamashita,
"The role of the methylammonium cation in the structural and electronic properties of 3D organic-inorganic perovskite halides: a DFT analysis including Spin Orbit Coupling", (**O.P.)**
"American Physical Society (APS), March Meeting 2014",
Mar 3-7th, 2014, Colorado Convention Center, Denver, Colorado, USA.

27) G. Giorgi, J.-I. Fujisawa, H. Segawa, K. Yamashita,
"The role of the inorganic cation MA ($CH_3NH_3^+$) in pseudocubic 3D $MAPbI_3$ organic-inorganic perovskites", (**P.P.)**
"5th JCS International Symposium on Theoretical Chemistry"
Dec 2-6th, 2013, Todai-ji Culture Center, Nara, JAPAN.

26) G. Giorgi, J.-I. Fujisawa, H. Segawa, K. Yamashita,
"Theoretical studies of organic-inorganic hybrid perovskites", (**O. P.)**
"55th Annual Meeting of The Electrochemical Society of Japan"
Tokyo Institute of Technology, September 27-29th, 2013, Okayama, Tokyo, JAPAN.

25) G. Giorgi, M. Palummo, A. Rubio, H. Segawa, K. Yamashita
"Minority surfaces of anatase & derived layered structures: optical signatures and functionalization in photovoltaics oriented applications", (**O. P.)**
"IMAMPC 2013, International Meeting on Atomic and Molecular Physics & Chemistry", Jul 2-5th 2013, Lille, FRANCE.

24) G. Giorgi, J.-I. Fujisawa, H. Segawa, K. Yamashita.
"Unravelling the Adsorption Mechanism of Aromatic and Aliphatic Diols on TiO_2 Surface: A DFT analysis", (**O. P.)**
"16th Annual Meeting of Japanese Theoretical Chemistry Society", Health Promotion Support Center, Fukuoka, 2013 May 15th-17th, JAPAN.

23) G. Giorgi, M. Palummo, L. Chiodo, A. Rubio, K. Yamashita.
"The nature of radiative transitions in 2D TiO_2 systems", **(P.P)**
"2012 MRS Fall Meeting & Exhibit" November 25-30th 2012, Hynes Convention Center, Boston, MA, USA.

22) G. Giorgi, M. Palummo, L. Chiodo, A. Rubio, K. Yamashita.
"The nature of radiative transitions in TiO_2-based nanosheets", **(P.P.)**
"ISSP-CMSI international workshop/symposium on MAterial Simulation in Petaflops era (MASP2012)", Institute of Solid State Physics, (ISSP), Workshop:
Jun 25th –Jul 1st and Jul 3rd-11th, 2012. Symposium: Jul 2nd, 12th, and 13th, 2012. Kashiwa Campus, The University of Tokyo, JAPAN.

21) G. Giorgi, M. Palummo, K. Yamashita.
"Excitons at the (001) surface of anatase: Spatial behavior and optical signatures" (**P.P.)**
"ASIAN-14. The 14th Asian Workshop on First-Principles Electronic Structure Calculations".
Oct 31st -Nov 2nd, 2011, The University of Tokyo, Tokyo, JAPAN.

20) G. Giorgi, M. Palummo, L. Chiodo, K. Yamashita
"Precursor optical excitations of photocatalysis at the (001) surface of TiO_2 anatase", (**P.P.)**
"WATOC 2011, 9th triennial congress of the World Association of Theoretical and Computational Chemists", Jul 17-22nd, 2011, Santiago de Compostela, SPAIN.

19) G. Giorgi, M. Van Schilfgaarde, A. Korkin, K. Yamashita
"Chemical origin of the gap bowing in $(GaAs)_{1-x}Ge_{2x}$ alloys: A combined DFT QSGW study", (**P.P.)**
"PACIFICHEM 2010, The International Chemical Congress of Pacific Basin Societies", Dec 15-20th, 2010, Honolulu, Hawaii, USA

18) G. Giorgi, M. Palummo, K. Yamashita
"On the excitonic effects on TiO_2 low-dimensional systems: a combined DFT+MBPT approach", (**O. P.)**
"4th Annual Meeting of Japanese Society of Molecular Science",
Sep 14-17th, 2010, Toyonaka Campus, Osaka University, Osaka, JAPAN

17) G. Giorgi, L.R.C.Fonseca, A. Korkin, K. Yamashita
"A combined DFT-scattering theory approach for transport properties calculation of HfO_2/Si/HfO_2 silicon-on-insulator FET", (**P.P.)**
"Nano and Giga Challenges in Electronics, Photonics and Renewable Energy- 14th Canadian Semiconductor Technology Conference" Symposium and Summer School, August 10-14th, 2009, Hamilton, Ontario, CANADA

16) G. Giorgi, A. Korkin, K. Yamashita
"Stress and strain effect analysis of ZrO_2 & HfO_2 interface with silicon", (**P. P.)**
"The Horiba International Symposium on Simulations and Dynamics for Nanoscale and Biological Systems" Mar 4-6th 2009, The University of Tokyo, Tokyo, JAPAN

15) G. Giorgi, X. Cartoixà, A. Sgamellotti, R. Rurali
"Mn-doped Si nanowires", (**P. P.)**
Cecam workshop - "Structural, electronic and transport properties of quantum wires", Jun 9-12th 2008, Lyon, FRANCE.

14) G. Giorgi, P. Belanzoni, G.F. Cerofolini, A. Sgamellotti
"On a metastable configuration at the H-terminated (100) Si surface", (**O. P.)**
"6th National Congress INSTM 2007", Jun 12-15th 2007, Perugia, ITALY.

13) G. Giorgi, P. Belanzoni, G.F. Cerofolini, A. Sgamellotti
"Anomalous" behavior of atomic silicon: a DFT approach to silicon surfaces", (**P.P.)**
"SAMIC2006-SYNTHESES AND METHODOLOGIES IN INORGANIC CHEMISTRY-From Molecules to Nanosystems", Dec 3-7th, 2006, Bressanone, ITALY.

12) G. Giorgi, A. Korkin, K. Yamashita
"Stress & strain at Si-HfO_2 interfaces", (**P.P.)**
"International COE Symposium for Young Scientist on Frontiers of Molecular Science", Aug 25-26th, 2006, Koshiba Hall, The University of Tokyo, Tokyo, JAPAN.

11) P. Belanzoni, ***G. Giorgi***, G.F. Cerofolini, A. Sgamellotti
"Studio teorico della reazione del silicio col carbonile", (**P.P.)**
"QUITEL2005, Congress for Theoretical Chemists of Latin Expression",
Oct 2-6th, 2005, Isla Margarita, VENEZUELA.

10) G. Giorgi, M. Deumal, M.A. Robb, M. Turnbull, C. Landee, J.J. Novoa
"Magnetic interaction of the 2-amino-5-nitropyridine tetrabromocuprates (MUJYOF): A f first principles *bottom-up* theoretical study", (**P.P.)**
"5th National Congress INSTM 2005", Sep 26-29th 2005, Geremeas- Maracalagonis (CA), ITALY.

9) P. Belanzoni, ***G. Giorgi***, G.F. Cerofolini, A. Sgamellotti
"The silicon chemistry: silicon carbonyls as a new class of inorganic compounds", (**P.P.)**
"5th National Congress INSTM 2005", Sep 26-29th, 2005, Geremeas-Maracalagonis (CA), ITALY.

8) G. Giorgi, P. Belanzoni, G.F. Cerofolini, A. Sgamellotti
"The new class of silicon-carbonyl compounds: a DFT approach", (**P.P.)**
"DFT2005 Conference", Sep 11-15th, 2005, Geneva, SWITZERLAND.

7) P. Belanzoni, ***G. Giorgi***, G.F. Cerofolini, A. Sgamellotti
"The silicon carbonyls: a new class of inorganic compounds", (**P.P.)**
"8th FIGIPAS. Meeting in Inorganic Chemistry", 2005 Jul, 6-9th, Athens, GREECE.

6) G. Giorgi, P. Belanzoni, G.F. Cerofolini, A. Sgamellotti
"Theoretical investigations on atomic-silicon cryptates in siloxanic networks", (**O.P.)**
"Nano and Giga Challenges in Microelectronics", Sept. 13-17th, 2004, Cracow, POLAND.

5) G. Giorgi, G.F. Cerofolini, N. Re, A. Sgamellotti
"Concerted vs. radical hydrosilylation mechanism in the uncatalyzed thermal functionalization of silicon surfaces by alkenes and alkynes", (**P.P.)**
"3rd Computational modeling and simulation of materials & Special Symposium Modelling and Simulating Materials Nanoworld", May 30th –June 4th, 2004, Acireale (CT), ITALY.

4) P. Belanzoni, ***G. Giorgi***, G.F. Cerofolini, A. Sgamellotti
"Atomic silicon in siloxanic matrices: a density functional approach" (**P. P.),**
"3rd Computational modeling and simulation of materials & Special Symposium Modelling and Simulating Materials Nanoworld", May 30th –June 4th, 2004, Acireale (CT), ITALY.

3) G. Giorgi, F. De Angelis, N. Re, A. Sgamellotti
"Theoretical investigations on mechanisms involved in hybrid integrated circuit building" (**O.P.),**
"International Conference on Computational Science (ICCS2003)",
June, 2-4th, 2003, Saint Petersburg, RUSSIAN FEDERATION.

2) G. Giorgi, F. De Angelis, N. Re, A. Sgamellotti
"Theoretical investigations on mechanisms involved in hybrid integrated circuit building", (**P.P.)**
"The 2002 Younger European Chemists' Conference Highlights of European Chemistry Research and R&D", Sep 30th–Oct 2nd 2002, Heidelberg, Germany.

1) G. Giorgi, N. Re, A. Sgamellotti
"Theoretical study on selective grafting mechanisms to systems containing silicon", (**O.P.)**
"International School of Liquid Crystals, 6th Workshop "New Challenges in Computational Modelling: Techniques for Processes, Molecular Systems and Anisotropic Materials",
Oct 25-28th, 2001, Erice (TP), ITALY

CONFERENCES & WORKSHOPS ORGANIZED

4. Psi-k workshop "2D Layered materials for opto-electronics: a theoretical/computational perspective",

   Dec 18-19th 2017, Italian Cecam Node, Rome, ITALY.

3. CECAM workshop: “THEORETICAL MODELLING AND SIMULATION OF PEROVSKITE-BASED SOLAR CELLS”,
   Aug 23rd- 25th, 2015, CECAM-HQ, Lausanne, SWITZERLAND.

2. "Computer modeling of materials at the nanoscale” - An introduction and hands-on tutorial with the QUANTUM ESPRESSO & YAMBO codes.

   Apr 23-26th, 2014, Sanjo Conference Hall. The University of Tokyo, Hongo Campus, Tokyo, JAPAN.

1. "CERC3 - Young Chemists' Workshop Modelling of Complex Systems",
   May 1st-4th, 2008 Perugia, ITALY (Local Organizing Staff