C U R R I C U L U M V I T A E

Luca Grisanti
date of birth: 29/08/1983

viale Miramare 55
34135 Trieste, Italy

e- mail: luca.grisanti@gmail.com,
grisanti@iom.cnr.it
lgrisant@irb.hr

mobile phone: +39 329 2136722

E D U C A T I O N & R E S E A R C H

Associate Researcher (December 2022 - now)

Consiglio Nazionale Ricerche – National Research Council (CNR), Trieste, Italy
Istituto Officina dei Materiali - Institute of Material Foundry (IOM), CNR-IOM@Trieste-SISSA

- *Research topics and interests.*. Biological matter and computational biophysics: architectures and dynamics of biological molecules and materials, from structure and dynamics to opto-electronic properties; Computational material science: modeling material properties ; Chemical physics and theoretical spectroscopy: computational description of excited states and optical properties in molecular and bio- materials, aggregates and molecules.

Associate Researcher (October 2018 – November 2022)
External collaborator (December 2022 – now)

Ruđer Bošković Institute (IRB), Zagreb, Croatia
Division of Theoretical Physics – Condensed Matter and Statistical Physics Laboratory

- *Research topics and interests.* Computational material science: modeling material properties from electronic structure to morphology and dynamics. Development of computational approaches for charges and excitons in molecular and hybrid materials, transport and role of electron-phonon coupling; Biological matter and computational biophysics. Chemical physics and theoretical spectroscopy.

Post-doctoral Research fellows / Assegno di ricerca (December 2016 – September 2018)

Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy
Condensed Matter Theory group

- *Research topics and interests.* Computational material science: electronic and optical properties in organic materials, organic molecules and bio-molecules. Solvation dynamics and environmental effects. Optical properties of organic dyes, relation with dynamical and structural properties. Computational biophysics for electronic and optical properties of polypeptides and related model systems.

Project involvement: project coordinated by industrial partner with an international network

Post-doctoral Research fellows (October 2013 – October 2016)

The “Abdus Salam” International Centre for Theoretical Physics (ICTP), Trieste, Italy
Section of Condensed Matter and Statistical Physics

- *Research topics and interests.* Computational material science: electronic and optical properties in organic materials and bio-materials. Computational biophysics: development of computational approaches to multi-scale modelling of polypeptides and related model systems, from electronic and optical properties, to structure and interaction with the environment.

Post-doctoral Research fellow (February 2011 – August 2013)

Université de Mons, Belgium

Laboratory for Chemistry of Novel Materials

- *Research topics and interests.* Organic molecular electronics: modelization and development of computational approaches for charge and exciton diffusion in organic molecular materials, role of the exciton-phonon coupling in exciton and charge transport, exciton and charge dynamic and localisation

European project involvement:

- MMM@HPC European Project (Multiscale Material Modelling on High Performance Computer Architectures - European Community FP7) (January 2012 – August 2013)
- ONE-P European Project (Organic Nanomaterials for Electronics and Photonics - European Community FP7) (Februrary 2011 – December 2011)

Ph.D. Studies (January 2008- December 2010)

PhD in Chemical Sciences, Dipartimento di Chimica G.I.A.F. (General, Inorganic, Analitic and Physical Chemistry Department) – University of Parma (Italy)

- Thesis title: "*CHARGE AND ENERGY TRANSFER IN FUNCTIONAL MOLECULAR MATERIALS: SPECTROSCOPY AND MODELS",* advisors: A. Girlando, A. Painelli
- PhD defended on 04-03-2011 at the University of Parma
- Research topics: molecular spectroscopy, study of linear and non-linear optical properties of molecules, aggregates, and molecular materials; measure, modelling, calculation and interpretation of optical response of such systems, environmental effect on electronic and optical properties, energy transfer and intermolecular interactions
- Short external PhD Stay:
  - JNCASR (Jawaharlal Nehru Centre for Advanced Scientific Research), Jakkur Campus (Bangalore, India) - Molecules To Materials Group (Theoretical Sciences Unit), supervisor: Prof. Swapan Pati (March-April 2010)
  - ICMAB–CSIC, Campus UAB Bellaterra (Barcelona) - Molecular Nanoscience and Organic Materials Department, supervisor: Prof. Jaume Veciana (April-May 2009)

Graduated Studies (2005 - 2007)

Title: Laurea specialistica in Chimica, curriculum: Chimica Fisica (Master/Second Level Deegre in Chemistry, Physical Chemistry curriculum) - Università degli Studi di Parma (Italy)

- Thesis Title: "*Materiali molecolari per applicazione avanzate: modellizzazione e caratterizzazione spettroscopica in un approccio bottom-up*" (Molecular Materials for advanced applications: modellization and characterization in a bottom-up approach), supervisors: Anna Painelli, Alberto Girlando
- Graduated on 28-09-2007, graduating mark: 110/110 e lode (Magna cum laude)
- Post-graduate short term contract (October-December 2007), Dipartimento di Chimica G.I.A.F. (General, Inorganic, Analitic and Physical Chemistry Department) – University of Parma (Italy)

Undergraduated Studies (2002 – 2005)

Title: Laurea in Scienze e Tecnologie Chimiche (Bachelor/First level deegre in Chemical Sciences and tecnologies) - Università degli Studi di Parma (Italy)

- Thesis Title "*Solvatocromismo e proprietà ottiche non lineari: uno studio sperimentale del 4-dimetilammino-4'-nitrostilbene*" (Solvatochormism and non linear optical properties: an experilmental study of 4-dimetilammino-4'-nitrostilbene), supervisors: Anna Painelli, Matteo Masino
- Bachelor of Science on 15-07-2005, mark: 110/100 e lode (Magna cum laude)

High School studies (1997 - 2002)

Title: "Maturità scientifica", Liceo Scientifico Statale "A. Moro" , Reggio Emilia, final mark 100 / 100

- School-work training (June - July 2001): summer training period, Quality Service Laboratory, IREN (ex-ENIA/AGAC), Reggio Emilia (Italy)

PUBLICATION LIST, CONTRIBUTIONS TO CONFERENCES AND SEMINARS

Peer Reviewed Articles - 34 published,
tot. citations WoS (on 32 papers)**: 939 H-index Wos: 17, H-index Google Scholar: 18**

1. "*Fluorescent Multifunctional Organic Nanoparticles for Drug Delivery and Bioimaging: A Tutorial Review*", G. Vargas-Nadal, M. Köber, A. Nsamela, F. Terenziani, C. Sissa, S.Pescina, F. Sonvico, A. M. Gazzali, H.A Wahab, L.Grisanti, M. Eugenia Olivera, M. Celeste Palena, M. Laura Guzman, L. Carolina Luciani-Giacobbe, A. Jimenez-Kairuz, N. Ventosa, I. Ratera, K. D. Belfield, B. M Maoz, Pharmaceutics, 14 (11), 2498 (2022)
2. *"Photoinduced Segregation Behavior in 2D Mixed Halide Perovskite: Effects of Light and Heat"* T. Lun Leung, Z. Ren, A. Asgher Syed, L. Grisanti, A. B. Djurišić, and J. Popović, *ACS Energy Lett.*, 7 (10) 3500–3508 (2022)
3. *"Non-Aromatic Fluorescence in Biological Matter: The Exception or the Rule?,* U. N. Morzan, G. Díaz Mirón, L. Grisanti, M. C. González Lebrero, G. S. Kaminski Schierle, A.Hassanalii*, J. Phys. Chem. B*, 126(38), 7203–7211 (2022)
4. *"Mixed Halide Ordering as a Tool for the Stabilization of Ruddlesden–Popper Structures"*, J..Ovčar, T. L. Leung, L. Grisanti, Ž. Skoko, M. Vrankić, K—H.Low, S. Wang, P.-Y.You, H. Ahn, I. Lončarić, A. B Djurišić, J. Popović, *Chem. Mater.* 34(10), 4286-4297 (2022)
5. "*Enhanced Light Emission Performance of Mixed Cation Perovskite Films—The Effect of Solution Stoichiometry on Crystallization*", F. Liu, X. Qin, B. Han, C. CS Chan, C. Ma, T. Lun Leung, W. Chen, Y. He, I. Lončarić, L. Grisanti, J. Ovčar, Ž. Skoko, Y. Shi, F. C. Chung Ling, M. R. Huqe, J. A. Zapien, S. Wang, C.-J. Su, U-. Jeng, K.Sing Wong, A. M. Ching Ng, M. Gu, J. Popović, A. B Djurišić *Adv. Opt. Mat.* 9 (21), 2100393 (2021)
6. "*Short hydrogen bonds enhance nonaromatic protein-related fluorescence*", A. D. Stephens, M. N. Qaisrani, M. T. Ruggiero, G. Díaz Mirón, U. N. Morzan, M. C. González Lebrero, S. T. E. Jones, E. Poli, A. D. Bond, P. J. Woodhams, E. M. Kleist, L. Grisanti, R. Gebauer, J. A. Zeitler, D. Credgington, A. Hassanali, and G. S. Kaminski Schierle. *Proc. Natl. Acad. Sci. U.S.A.* 118 (21) e2020389 (2021); pre-print *Biorxiv* https://www.biorxiv.org/content/10.1101/2020.01.22.915306v2
7. "*Discovery of a natural cyan blue: A unique food-sourced anthocyanin could replace synthetic brilliant blue*" P. R. Denish, J.-A. Fenger, R. Powers, G. T. Sigurdson, L. Grisanti, K. G. Guggenheim, S. Laporte, J. Li, T. Kondo, A. Magistrato, M. P. Moloney, M. Riley, M. Rusishvili, N. Ahmadiani, S. Baroni, O. Dangles, M. Giusti, T. M. Collins, J. Didzbalis, K. Yoshida, J. B. Siegel and R. J. Robbins, *Science Advances*, 7(15), eabe7871 (2021)
8. "*Understanding Förster Energy Transfer through the Lens of Molecular Dynamics*", M. Anzola, C. Sissa, A. Painelli, A. Hassanali, L. Grisanti, *J. Chem. Theor. Comput.* 16(12) 7281-7288 (2020)
9. "*Toward understanding optical properties of amyloids: a reaction path and nonadiabatic dynamics study*" L. Grisanti, M. Sapunar, A. Hassanali, N. Došlić, *J. Am. Chem. Soc.* 142 (42), 18042-18049 (2020)
10. "*Phase control for quasi-2D blue emitters by spacer cation engineering*" H. W. Tam, T. L. Leung, W. Sun, F. Liu, C. Ma, K. S. Wong, I. Lončarić, L. Grisanti, J. Ovčar, Ž. Skoko, J. Popović, A. B Djurišić, *J. Mater. Chem. C* 8, 11052-11060 (2020)
11. "*Mixed Spacer Cation Stabilization of Blue-Emitting n = 2 Ruddlesden–Popper Organic–Inorganic Halide Perovskite Films*", T. L. Leung, H. W. Tam, F. Liu, J. Lin, A. M. Ching Ng, W. K. Chan, W. Chen, Z. He, I. Lončarić, L. Grisanti, C. Ma, K. S. Wong, Y. S. Lau, F. Zhu, Ž. Skoko, J. Popović, A . B Djurišić, *Adv. Opt. Mat.* 8 (4), 1901679 (2020)
12. "*Structural and dynamical heterogeneities at glutamine–water interfaces*". M.N. Qaisrani, L. Grisanti, R. Gebauer, A. Hassanali, *Phys. Chem. Chem. Phys.* 21 (29), 16083-16094 (2019)

13. "*Unraveling the molecular mechanisms of color expression in anthocyanins*", M. Rusishvili, L. Grisanti, S. Laporte, M. Micciarelli, M. Rosa, R. Robbins, T. Collins, A. Magistrato, and S. Baroni, *Phys. Chem. Chem. Phys.* 21, 8757-8766 (2019)
14. "*Low Energy Optical Excitations as an Indicator of Structural Changes Initiated at the Termini of Amyloid Proteins*", J. KwangHyok, Y. T. Azar, L. Grisanti, A. D. Stephens; S. T. E. Jones, D. Credgington, G. Kaminski and A. Hassanali, *Phys. Chem. Chem. Phys.* 21 (43), 23931-23942 (2019); pre-print: *ChemRxiv* https://doi.org/10.26434/chemrxiv.7215065.v1 (2018)
15. "*Understanding the Quantum Mechanical Properties of Hydrogen Bonds in Solvated Biomolecules from Cluster Calculations*", N. Ansari, J. KwangHyok, L.Grisanti and A. Hassanali, *J. Mol. Liq. 263*, 501-509 (2018)
16. *"Hydrogen Bond Networks and Hydrophobic Effects in the Amyloid β_{30-35} Chain in Water: A Molecular Dynamics Study"*, J. KwangHyok; L. Grisanti, A. Hassanali, *BioRxiv* https://doi.org/10.1101/090092 and *J. Chem. Inf. Model. 57(7)*, 1548-1562 (2017)
17. *"A Computational Study on how Structure Influences Optical Properties in Model Crystal Structures of Amyloid Fibrils"*, L. Grisanti, D. Pinotsi, R. Gebauer, G. S. Kaminski Schierle and A. A. Hassanali, *Phys. Chem. Chem. Phys 19*, 4030-4040 (2017)
18. *"Light-enhanced liquid-phase exfoliation and current photoswitching in graphene–azobenzene composites"* M. Döbbelin, A. Ciesielski, S. Haar, S. Osella, M. Bruna, A. Minoia, L. Grisanti, T. Mosciatti, F. Richard, E. A. Prasetyanto, L. De Cola, V. Palermo,R. Mazzaro, V. Morandi, R. Lazzaroni, A. C. Ferrari, D. Beljonne, P. Samorì *Nature Communications 7*, 11090 (2016)
19. *"Proton delocalization and structure-specific fluorescence in hydrogen bond-rich protein structures"* D. Pinotsi, L. Grisanti, P. Mahou, R. Gebauer, C. Kaminski, A. Hassanali and G. Kaminski Schierle, *J. Am. Chem. Soc. 138 (9),* 3046–3057 (2016)
20. *"Influence of the supramolecular order on the electrical properties of 1D coordination polymers based materials",* C. Musumeci, S. Osella, L. Ferlauto, D. Niedzialek, L. Grisanti, S. Bonacchi, A.Jouaiti, S. Milita, A. Ciesielski, D. Beljonne, M. W. Hosseini, P. Samorì, *Nanoscale 8*, 2386-2394 (2016)
21. *"Toward Fast and Accurate Evaluation of Charge On-Site Energies and Transfer Integrals in Supramolecular Architectures Using Linear Constrained Density Functional Theory (CDFT)-Based Methods"* L. E. Ratcliff, L. Grisanti, L. Genovese, T. Deutsch, T. Neumann, D. Danilov, W. Wenzel, D. Beljonne and J. Cornil, *J. Chem. Theory Comput. 11*, 2077–2086 (2015)
22. "*Roles of local and nonlocal electron-phonon couplings in triplet exciton diffusion in the anthracene crystal*" L. Grisanti, Y. Olivier, L. Wang, S. Athanasopoulos, D. Beljonne and J. Cornil, *Phys. Rev. B 88*, 035450 (2013)
23. *"Intra- and Intermolecular Charge Transfer in Aggregates of Tetrathiafulvalene-Triphenylmethyl Radical Derivatives in Solution"* J. Guasch, L. Grisanti, M. Souto, V. Lloveras, J. Vidal-Gancedo, I. Ratera, A. Painelli, C. Rovira and J. Veciana, *J. Am. Chem Soc. 135* 6958–6967 (2013)
24. *"Bistability of Fc-PTM-based dyads: The role of the donor strength"* J. Guasch, L. Grisanti, S. Jung, D. Morales, G. D'Avino, M. Souto, X. Fontrodona, A. Painelli, F. Renz, I. Ratera and J. Veciana, *Chem. Mat.* 25(5) 808-814 (2013)
25. "*Tuning the Nature of the Fluorescent State: A Substituted Polycondensed Dye as a Case Study"* C. Sissa, V. Calabrese, M. Cavazzini, L. Grisanti, F. Terenziani, S. Quici and A. Painelli *Chem.-Eur. J.* 19(3), 924-935 (2013)
26. "*Interaction of charge carriers with lattice and molecular phonons in crystalline pentacene"* A. Girlando, L. Grisanti, M. Masino, A. Brillante, R. G. Della Valle and E. Venuti *J. Chem. Phys.* 135, 084701 (2013)
27. "*Induced Self-Assembly of a Tetrathiafulvalene-Based Open-Shell Dyad through Intramolecular Electron Transfer"* J. Guasch, L. Grisanti, V. Lloveras, J. Vidal-Gancedo, M. Souto, D. C. Morales, M. Vilaseca, C. Sissa, A. Painelli, I. Ratera, C. Rovira and J. Veciana *Angew. Chem. Int. Ed. Engl. 51*(44), 11024-8 (2012***)***
28. *"Polar Fluorenes and Spirobifluorenes: Fluorescence and Fluorescence Anisotropy Spectra*" L. Grisanti, F. Terenziani, C. Sissa, M. Cavazzini, F. Rizzo, S. Orlandi and A. Painelli *J. Phys. Chem. B 115* (39), 11420–11430 (2011)
29. "*Dimers of polar chromophores in solution: role of excitonic interactions in one- and two-photon absorption properties"* F. Todescato, I. Fortunati, S. Carlotto, C. Ferrante, L. Grisanti,

C. Sissa, A. Painelli, A. Colombo, C. Dragonetti and D. Roberto *Phys. Chem. Chem. Phys.* 13, 11099-11109 (2011)

30. *"Peierls and Holstein carrier-phonon coupling in crystalline rubrene"* A. Girlando, L. Grisanti, M. Masino, I. Bilotti, A. Brillante, R. G. Della Valle, and E. Venuti, *Phys. Rev. B 82*, 035208 (2010)
31. *"Enhancing the Efficiency of Two-Photon Absorption by Metal Coordination"* L. Grisanti, C. Sissa, F. Terenziani, A. Painelli, D. Roberto, F. Tessore, R. Ugo, S. Quici, I. Fortunati, E. Garbin, C. Ferrante, R. Bozio*, Phys. Chem. Chem. Phys. 11* (41), 9450-9457 (2009)
32. *"Cooperativity from electrostatic interactions: understanding bistability in molecular crystals"* G. D'Avino, L. Grisanti, A. Painelli, J. Guasch, I. Ratera and J. Veciana *CrystEngComm* 11, 2040 – 2047 (2009)
33. *"Essential State Models for Solvatochromism in Donor−Acceptor Molecules: The Role of the Bridge*" L. Grisanti, G. D'Avino, A. Painelli, J. Guasch, I. Ratera and J. Veciana, *J. Phys. Chem. B 113* (14)*,* 4718–4725 *(*2009*)*
34. *"Bistability in Fc-PTM Crystals: The Role of Intermolecular Electrostatic Interactions"* G. D'Avino, L. Grisanti, J. Guasch; I. Ratera, J. Veciana and A. Painelli, *J. Am. Chem. Soc.* 130 (36), 12064-12072 (2008*)*

Contributions to scientific conferences/schools as presenting author (oral presentation)

- Luca Grisanti
  Multiscale Modeling of Organic and Bio-materials: Energy Transfer and Molecular Excitons
  Computational Chemistry Day 2022, Ruđer Bošković Institute (Zagreb), 27/09/2022 (**as invited speaker**)
- Luca Grisanti, M. Anzola, C. Sissa, A. Painelli, A. Hassanali
  Förster resonance energy transfer through the lens of molecular dynamics
  ACS Spring 2021 technical program – COMP division live presentation, online, 5-30/04/2021
- Luca Grisanti, M. Rusishvili, S. Laporte, A. Magistrato, S. Baroni
  Structure-function relation in the color expression of natural dyes: a computational study of Anthocyanins
  9th European Symposium on Computing π-Conjugated Compounds, Naples (Italy), 11-13/02/2018
- Luca Grisanti, M. Rusishvili, S. Laporte, A. Magistrato, S. Baroni
  Predicting the color of natural dyes using quantum mechanics, statistical physics, and high-performance computing
  MaX Conference on the Materials Design Ecosystem at the Exascale: High-Performance and High-Throughput Computing, Trieste (Italy), 29-31/01/2018 (**as invited speaker**)
- Luca Grisanti, D. Pinotsi, R. Gebauer, G. S. Kaminski Schierle, A. Hassanali
  Computational studies of structural and electronic properties in Amyloids: from a single chain in solution to crystals
  MOLIM "Molecules in motion" 2nd general meeting, Dubrovnik (Croatia) 10-12/10/2016 (in the "Young Research Meeting" section)
- Luca Grisanti, D. Pinotsi, R. Gebauer, M. Sapunar, A. Ponzi, N. Došlić, G. S. Kaminski Schierle, A. Hassanali
  Structure-related fluorescence and proton delocalization in Amyloid Proteins
  MIPOMAT Workshop "Innovative Surfaces and Materials", Primošten (Croatia) 28-31/08/2016 (**as invited speaker**)
- Luca Grisanti, D. Pinotsi, R. Gebauer, M. Sapunar, N. Došlić, G. S. Kaminski Schierle, A. Hassanali
  Excited states in amyloid proteins: proton transfer and intrinsic fluorescence
  Workshop on Spectroscopy and Dynamics on Multiple Potential Energy Surfaces - Telluride Science Research Center, Telluride (United States), 18-22/07/2016
- Luca Grisanti, L. E. Ratcliff, L. Genovese, T. Deutsch, T. Neumann, D. Danilov, W. Wenzel, D. Beljonne, and J. Cornil

A Constrained Density Functional Theory (CDFT)-Based Method for Charge On-Site Energies and Transfer Integrals in Host-Guest Molecular Architectures
7th European Symposium on Computing π-Conjugated Compounds, Bordeaux (France), 11-13/02/2016

- Luca Grisanti
Modeling optical properties in amyloid proteins: proton delocalization and structure-related fluorescence
12th ETSF Young Researchers' Meeting "Challenges in ab initio modelling of materials and molecules" - Paris (France), 1-5/06/2015
- Luca Grisanti
Charge Transfer States In Devices: The Case Of Triplet Transport
CECAM Workshop "Charge Transfer Modeling in Chemistry: new methods and solutions for a long-standing problem" 7-10/04/2015, Paris (France)
- Luca Grisanti, G D'Avino, L. Muccioli, Y. Olivier, L. J. Wang, J. Cornil and D. Beljonne
Computational insights on the charge carrier dynamics in oligothiophenes
"5th European symposium on Computing π-Conjugated systems (CPiC5)", Linköping (Sweden), 5-7/02/2014
- Luca Grisanti and I. Kondov
Workflows in organic electronic: Polymer Based Devices & OLED
"Mapper Summer School on Distributed Multiscale Computing", Barcelona (Spain), 3-4 June 2013
- Luca Grisanti
Modelling the transport of excitons and charges in molecular materials: a combined computational approach
FNRS meeting "Calcul Intensif" ((Belgian Agency for Scientific Research, HPC meeting), 19/04/2013, Namur (Belgium)
- Luca Grisanti, Y. Olivier, S. Athanasopoulos, D. Beljonne and J. Cornil
Modeling triplet diffusion in oligoacene crystals: a combined quantum-chemical and Monte Carlo approach
"Third Symposium on Computing Pi-Conjugated Compounds (CPiC3)", Mons (Belgium), 2-4 February 2012
- Luca Grisanti, G. D'Avino, A. Painelli, J. Guasch, I. Ratera, J. Veciana
Electrostatic interactions in Ferrocene-PTM crystal: a new concept of bistability
ESMolNa2008, Gandia (E), 26-30 Oct. 2008

Contributions to scientific conferences/schools as presenting author (poster presentation):

- L. Savi, A. Painelli, Luca Grisanti
Hybrid modeling of molecular excitons in quinacridone crystals
Psi-k conference, EPFL, Lausanne (Switzerland), 22-25/08/2022
- Luca Grisanti, L. Savi, A. Painelli
From molecular electronic states to molecular excitons in quinacridone crystals
25th International Conference on the Chemistry of the Organic Solid State (ICCOSS XXV), Ohrid, North Macedonia, 03-08/07/2022
- Luca Grisanti, L. Savi, A. Painelli
From molecular electronic states to molecular excitons in quinacridone crystals
12th Symposium on Computing π-Conjugated Compounds, Grenoble, France, 13-14/05/2022
- Luca Grisanti, M. Sapunar, A. Hassanali, N. Došlić
Deciphering optical properties of amyloids: A reaction path and nonadiabatic dynamics study"
ACS Spring 2021 – PHYS division poster session, online, 5-30/04/2021
- Luca Grisanti, M. Anzola, C. Sissa, A. Painelli, A. Hassanali
Förster Resonance Energy Transfer through Molecular Dynamics
RSC Faraday joint interest group conference 2021, online, 29-31/03/2021
- Luca Grisanti, N. Qaisrani, R. Gebauer, G. Kaminski Schierle and A. Hassanali
Structural, optical and electronic properties of H-bond rich biological matter
Solid-State Science & Research, 27-29/06/2019, Zagreb, Croatia
- Luca Grisanti, M. Rusishvili, S. Laporte, A. Magistrato and S. Baroni,
Structure and color expression in anthocyanin-based natural dyes: a computational insight

Computational Chemistry Day, Faculty of Pharmacy and Biochemistry, *Zagreb, 11/05/2019*

- Luca Grisanti, M. Rusishvili, S. Laporte, A. Magistrato and S. Baroni
  Color properties of materials: a multi-scale computational approach for anthocyanins dyes in solution
  10th Symposium on Computing π-Conjugated Compounds, Valencia, 1-2/02/2019
- Luca Grisanti, M. Rusishvili, S. Laporte, A. Magistrato, S. Baroni
  Computational insight on the relation between structure and color expression in anthocyanin-based natural dyes and their metal complexes
  19th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods, ICTP Trieste (Italy), 9-11/01/2019
- Luca Grisanti, M. Rusishvili, S. Laporte, A. Magistrato, S. Baroni
  Color properties of materials: a multi-scale computational approach for anthocyanins dyes in solution
  Game of Materials, Dubrovnik (Croatia) 30/10-2/11/2018
- Luca Grisanti, M. Rusishvili, S. Laporte, A. Magistrato, S. Baroni
  Absorption properties of natural dyes: a multi-scale computational approach for anthocyanins
  Photoinduced Processes in Embedded Systems - PPES2018, Pisa (Italy), 24-27/06/2018
- Luca Grisanti, D. Pinotsi, R. Gebauer, A. Hassanali, G. S. Kaminski Schierle
  Fluorescence beyond conjugation: structure-related fluorophore and proton delocalization in amyloid protein
  7th European Symposium on Computing π-Conjugated Compounds, Bordeaux (France), 11-13/02/2015
- Luca Grisanti, Y. Olivier, S. Athanasopoulos, D. Beljonne and J. Cornil
  Modeling triplet exciton diffusion in molecular crystals: a combined quantum-chemical and Monte Carlo approach
  "10th International Conference on Excitonic Processes in Condensed Matter, Nanostructured and Molecular Materials" (EXCON 2012), Groningen (NL) 2-6 July 2012
- Luca Grisanti, Y. Olivier, S. Athanasopoulos, D. Beljonne and J. Cornil,
  Characterization of triplet diffusion in organic semiconductors: a combined quantum-chemical and Monte-Carlo approach
  "Photovoltaics at the nanoscale" Hasselt (Belgium), 24-28 October 2011
- Luca Grisanti, C. Sissa, F. Terenziani ed A. Painelli
  CT chromophores and complexes: spectra and models
  "X Giornata della Chimica dell'Emilia Romagna", Parma (I), 26 November 2010
- Luca Grisanti, C. Sissa, F. Terenziani ed A. Painelli
  CT chromophores and complexes: spectra and models
  "Emergent Properties and Novel Behavior at the Nanoscale" School and Conference, Bangalore, (India), 19-27 April 2010 (poster communication)
- Luca Grisanti, C. Sissa, G. D'Avino, F. Terenziani ed A. Painelli
  Theoretical state models for functional molecular material: crossing the line between theory and experiment
  "IX Giornata della Chimica dell'Emilia Romagna", Bologna (I), 4 Dec. 2009
- Luca Grisanti, C. Sissa, G. D'Avino, F. Terenziani ed A. Painelli
  Essential state models for functional molecular material: crossing the line between theory and experiment
  Molecular Properties '09, Oslo (N), 18-21 June 2009
- Luca Grisanti**,** G. D'Avino, A. Painelli, J. Guasch, I. Ratera, J. Veciana
  Electrostatic interactions in Ferrocene-PTM crystal: a new concept of bistability
  ElecMol08, Grenoble (F), 8-12 Dec.. 2008

Seminars on scientific visits:

- Institut Néel / CNRS, Grenoble (France), 17 May 2022
  Interactions in molecular systems and multiscale modeling of organic and bio-materials: the case of energy transfer
- NJIT, Newark (United States), 4 May 2022
  Multiscale modeling of molecular systems and materials: the case of energy transfer
- University of Oslo (Norway), 9 February 2018

Structure-function relation in the color expression of natural dyes: a multi-level computational study of Anthocyanins

- Ohio State University – Columbus (United States), 2 August 2016
  Amyloid proteins: proton transfer and intrinsic fluorescence
- Rudjer Boskovic Institute - Zagreb (Croatia), 22 February 2016
  Structure-related fluorophore and proton delocalization in amyloid proteins
- Università di Parma (Italy), 1 October 2015
  Optical properties in amyloid proteins: structure-related fluorescence and proton delocalization

PROJECTS AND ACADEMIC SERVICES

Principal Investigator of **"**Hybrid modeling for excited states in novel molecular materials: from optical properties to exciton dynamics" (HYMO4EXNOMOMA), Croatian Science Fundation (2021-2025), https://sites.google.com/view/hymo4exnomoma

Team member of "Multifunctional nanocarriers for nonlinear microscopy: new tools for biology and medicine" (Micro4Nano), EU H2020-MSCA-RISE (2021-2025)

Team member of "Exploring halide 2D and quasi-2D perovskites: from rational structural design to enhanced efficiency and stability", HRZZ PZS-2019-02-2068 (2019-2023), https://jasminkapopovic5.wixsite.com/2dperoexplore

National **Academic Qualification as Associate Professor** in Condensed Matter Theory (Abilitazione Scientifica Nazionale, II Fascia, 02/B2 - FISICA TEORICA DELLA MATERIA) 11/05/2021- 11/05/2030

National **Academic Qualification as Associate Professor** in Physical Chemistry (Abilitazione Scientifica Nazionale, II Fascia, 03/A2 - MODELLI E METODOLOGIE PER LE SCIENZE CHIMICHE) 31/07/2018 - 31/07/2024

Principal investigator on accepted proposal for peer-review beamtime allocation, projects at CERIC & Elettra Synchrotron– Trieste (Italy), 2018 , 2021 and 2022

Conference organization (main proposer)**:** "Light-matter Interactions from scratch: Theory and Experiments at the Border with Biology", school and workshop 22-25/11/2021, online - ICTP funded activity

Symposium organization (main organizer) 11th European Symposium of "Computing pi-conjugated Compounds" , 30-01/02/2020, IRB, Zagreb (Croatia)

Conference organization (local organizer)**:** "Conference On The Complex Interactions Of Light And Biological Matter: Experiments Meet Theory", 21-25/05/2018, ICTP, Trieste (Italy)

Conference/School Support: "Summer School on Atomistic Simulation Techniques for Material Science, Nanotechnology, and Biophysics" 14-30/06/2017, SISSA, Trieste (Italy)

Member of PhD evaluation committées: Miha Gunde (Univ. Toulose – France, 2021), María Irene Badía Domínguez (Univ. Malaga – Spain, 2022)

Refereeing activities: Regular reviewer of scientific journals (APS, ACS, MDPI)

TEACHING AND TUTORING ACTIVITIES

Advising of 1 PhD student (2021-2025) – IRB, Zagreb
Supervision of a student in the frame of the HYMO4EXNOMOMA project (Croatian Science Fundation)

Advising of Postdoctoral fellowship (2022-2024) – IRB, Zagreb

Organiser and Lecturer for a 1-day Student tutorial (April 2022) – NJIT, Newark, US
"How To Approach Computer Simulations For Molecules And Materials: From Theory To Practice"

Lecturer for a PhD Student short course (10hs, December 2019) – University of Parma, Italy
"Introduction to Molecular Dynamics Simulations" Theory and Hands-on

Co-tutoring of PhD students (2017) – SISSA, Trieste and co-tutoring Diploma Postgraduate Students (2016-2017) – ICTP
Supervision and co-tutoring of student projects

Teaching assistant for courses of Postgraduate Diploma Programme (2015-2016) – ICTP, Trieste
Support activities for practical classes and exercise - "Numerical Methods" courses

Exercise Tutor for courses of Chemistry (2012/2013) – Université de Mons
Support activities for practical classes (computer simulations) - Physical Chemistry courses

Exercise Tutor and Laboratory assistant for courses of Chemistry and Material Science (2008/2009 and 2009/2010) – Università di Parma.
Support activities for practical classes and exercise - Physical Chemistry courses

Tutor for Chemistry course students (Academic years 2008/2009 and 2009/2010) - Facoltà di Scienze MM. FF. NN. (Faculty of Mathematical, Physical and Natural Sciences) – Università di Parma.
Tutor for the help of undergraduated and graduated students of Chemistry courses.

"Stage Estivi a Chimica" (June 2010, June-July 2009 and June 2008), Dipartimento di Chimica G.I.A.F. (Università di Parma)
Tutor of groups of high school students, project "Lauree Scientifiche". Subject: "Luce e Molecole" (Light and Molecules)

AWARDS

- Awarded as best undergraduate student in Chemistry for academic years 2002-2003 and 2003-2004 – University of Parma

LANGUAGES

Italian: native language
English: fluent understanding, speaking, reading and writing
French: fluent understanding, speaking and reading, very good writing
Spanish: very good understanding, good speaking and reading, basic writing
Croatian: only basic notions

I N F O R M A T I C S K I L L S

- *Operative System:* Unix/Linux and Windows-based;
- *Scientific Programming/scripting:* Fortran, Python (and related scientific extension numpy, scipy, matplotlib), Matlab/Octave and similar object-oriented codes for data analysis, and plotting;
- *Scripting / Unix shell programming:* bash/(t)csh
- *Quantum-chemistry and Condensed matter oriented packages:* ab-initio calculation program (Gaussian, ADF, NW-chem, ORCA and similar; CP2K and Quantum-ESPRESSO), semi-empirical (MOPAC and similar), molecular dynamics engines: Gromacs, Lammps
- *Package for molecular representations:* Jmol, Pymol, VMD

S C I E N C E C O M M U N I C A T I O N

- Communication (also as Oral Contribution to EGU 2019, Wien, Austria, 7-12 April 2019): “Topi da laboratorio: performing the science communication through theatre. ”, R. Nogherotto, D. Tenze, R. Cucini, T. Gasparetto, L. Grisanti, I. Persico, L. Pizzutti, S. Rossi , *Geophysical Research Abstracts* 21 (2019)
- Dissemination and science communication skills:
  - theatre & science project “Topi da Laboratorio”, performances: Teatro Miela - Trieste, (2017 and 2018), “Science Next Festival” (Trieste, 2016 and 2019), “Festival della Scienza di Genova” (2018), “Malnisio Science Festival” (2019) and “Isola di Einstein” (2019)
  - individual science dissemination performances: FameLab (Trieste – 2015, 2016) and Immaginario Scientifico (2019)
  - guide and scientific assistant for visitors, school classes and general public: “Science Next Festival” (Trieste, 2016), Trieste Mini Maker Faire (Trieste – 2015-2016) and Science Picnic (Trieste, 2016), “Science Next” Festival (Trieste - 2014), Science Exhibition “L’energia nelle tue mani” (2009 – Parma), summer activites for high school students, subject: “Light and Molecules”(2008-2010 – University of Parma)
- Other theatre activities, acting classes and workshops (2012-2018)

28th December 2022