Gaia Camisasca

ELENCO DELLE PUBBLICAZIONI E DELLA TESI DI DOTTORATO PRESENTATE

Pubblicazioni:

1) Iorio, A., **Camisasca, G.**, Gallo, P. “Slow dynamics of hydration water and the trehalose dynamical transition” (2019) Journal of Molecular Liquids, 282, pp. 617-625.

2) Perakis, F., **Camisasca, G.**, Lane, T.J., Späh, A., Wikfeldt, K.T., Sellberg, J.A., Lehmkühler, F., Pathak, H., Kim, K.H., Amann-Winkel, K., Schreck, S., Song, S., Sato, T., Sikorski, M., Eilert, A., McQueen, T., Ogasawara, H., Nordlund, D., Roseker, W., Koralek, J., Nelson, S., Hart, P., Alonso-Mori, R., Feng, Y., Zhu, D., Robert, A., Grübel, G., Pettersson, L.G.M., Nilsson, A. “Coherent X-rays reveal the influence of cage effects on ultrafast water dynamics article” (2018) Nature Communications, 9 (1), art. no. 1917.

3) **Camisasca, G.**, Iorio, A., De Marzio, M., Gallo, P. “Structure and slow dynamics of protein hydration water” (2018) Journal of Molecular Liquids, 268, pp. 903-910.

4) Mariedahl, D., Perakis, F., Späh, A., Pathak, H., Kim, K.H., **Camisasca, G.**, Schlesinger, D., Benmore, C., Pettersson, L.G.M., Nilsson, A., Amann-Winkel, K. “X-ray Scattering and O-O Pair-Distribution Functions of Amorphous Ices” (2018) Journal of Physical Chemistry B, 122 (30), pp. 7616-7624.

5) **Camisasca, G.,** De Marzio, M., Rovere, M., Gallo, P. “High density liquid structure enhancement in glass forming aqueous solution of LiCl” (2018) Journal of Chemical Physics, 148 (22), art. no. 222829.

6) De Marzio, M., **Camisasca, G.,** Rovere, M., Gallo, P. “Fragile to strong crossover and Widom line in supercooled water: A comparative study” (2018) Frontiers of Physics, 13 (1), art. no. 136103.

7) **Camisasca, G**., De Marzio, M., Rovere, M., Gallo, P. “Slow dynamics and structure of supercooledwater in confinement” (2017) Entropy, 19 (4), art. no. 185.

8) De Marzio, M., **Camisasca, G.,** Rovere, M., Gallo, P. “Microscopic origin of the fragile to strong crossover in supercooled water: The role of activated processes” (2017) Journal of Chemical Physics, 146 (8), art. no. 084502.

9) De Marzio, M., **Camisasca, G.,** Conde, M.M., Rovere, M., Gallo, P. “Structural properties and fragile to strong transition in confined water” (2017) Journal of Chemical Physics, 146 (8), art. no. 084505.

10) **Camisasca, G.,** De Marzio, M., Corradini, D., Gallo, P. “Two structural relaxations in protein hydration water and their dynamic crossovers” (2016) Journal of Chemical Physics, 145 (4), art. no. 044503.

11) De Marzio, M., **Camisasca, G.,** Rovere, M., Gallo, P. “Fragile-to-strong crossover in supercooled water: A comparison between TIP4P and TIP4P/2005 models” (2016) Nuovo Cimento della Societa Italiana di Fisica C, 39 (3), art. no. 302.

12) De Marzio, M., **Camisasca, G.,** Rovere, M., Gallo, P. “Mode coupling theory and fragile to strong transition in supercooled TIP4P/2005 water” (2016) Journal of Chemical Physics, 144 (7), art. no. 074503.

Tesi della tesi di dottorato:

“Slow Dynamics of Supercooled Water in Biological and Glass Forming Solutions - Insights from Molecular Dynamics”

Data: 23/04/19

Elenco pubblicazioni

Il candidato Federico Carollo presenta le seguenti pubblicazioni:

P1) F. Carollo, E. Gillman, H. Weimer, I. Lesanovsky, “Quantum contact process”, arXiv:1902.04515 (2019). Submitted to *Phys. Rev. Lett.*

P2) F. Carollo, R. L. Jack, J. P. Garrahan, “Unravelling the large deviation statistics of Markovian open quantum systems”, *Phys. Rev. Lett.***122** – 130605 (2019).

P3) F. M. Gambetta, F. Carollo, M. Marcuzzi, J. P. Garrahan, I. Lesanovsky, “Discrete time crystals in the absence of manifest symmetries or disorder in open quantum systems”, *Phys. Rev. Lett.* **122,** 015701 (2019).

P4) F. Carollo, J. P. Garrahan, I. Lesanovsky, C. Pérez-Espigares, “Fluctuating hydrodynamics, current fluctuations, and hyperuniformity in boundary-driven open quantum chains”, *Phys. Rev. E* **96** – 052118 (2017).

P5) F. Carollo, J. P. Garrahan, I. Lesanovsky, “Current fluctuations in boundary-driven quantum spin chains”, *Phys. Rev. B* **98**, 094301 (2018).

P6) F. Carollo, J. P. Garrahan, I. Lesanovsky, and C. Pérez-Espigares, “Making rare events typical in Markovian open quantum systems”, *Phys. Rev. A (R)* **98**, 010103 (2018).

P7) F. Benatti, F. Carollo, R. Floreanini, H. Narnhofer, “Quantum spin chain dissipative mean-field dynamics”, *J. Phys. A: Math. Theor.* **51**, 325001 (2018).

P8) C. Pérez-Espigares, F. Carollo, J. P. Garrahan and P. I. Hurtado, “Dynamical criticality in open system: non-perturbative physics, microscopic origin and direct observation” *Phys. Rev. E* **98** – 060102 (R) (2018).

P9) L. M. Vasiloiu, F. Carollo, M. Marcuzzi, J. P. Garrahan, “Strong zero modes in a class of generalised Ising spin ladders with plaquette interactions”, arXiv:1901.10211 (2019). Submitted to *Phys. Rev. B.*

P10) L. M. Vasiloiu, F. Carollo, and J. P. Garrahan, “Enhancing correlation times for edge spins through dissipation”**,** *Phys. Rev. B*, **98** – 094308 (2018).

P11) F. Benatti, F. Carollo, R. Floreanini, and H. Narnhofer, “Quantum fluctuations in mesoscopic systems”, *J. Phys. A: Math. Theor.* **50**, 423001 (2017).

P12) F. Benatti, F. Carollo, and R. Floreanini, “Dissipative entanglement of quantum spin fluctuations”**,** J. Math. Phys. **57**, 062208 (2016).

TESI) Tesi di Dottorato, Università di Trieste: F. Carollo ”Quantum Fluctuations and Entanglement in Mesoscopic Systems”

ELENCO PUBBLICAZIONI (12 MAX)

Recent developments of the ABINIT software package
X. Gonze, F. Jollet, F. Abreu Araujo, D. Adams, B. Amadon, T. Applencourt, … F. Da Pieve et al.,
Computer Physics Communications 205, 106 (2016) Impact Factor: 3.635

Casting light on the darkening of historical paintings
F. Da Pieve, C. Hogan, M. Radepont, F. Vanmeert, M. Cotte, J.Verbeeck, K. Janssens, D. Lamoen X. Gonze and G.Van Tendeloo
Phys. Rev. Lett. 111, 208302 (2013) Impact Factor: 7.645

Origin of magnetism and quasiparticles properties in Cr-doped TiO2
F. Da Pieve, S. Di Matteo, T. Rangel, M. Giantomassi, D. Lamoen, G.-M. Rignanese and X. Gonze,
Phys. Rev. Lett. 110, 136402 (2013) Impact Factor: 7.645

Analysis of the Local Boron Environment in Boron-doped Nanocrystalline Diamond Films, S.Turner, Y. Lu, S. D. Janssens**,** F. Da Pieve, D. Lamoen, J. Verbeeck, K. Haenen, P. Wagner and G. Van Tendeloo
Nanoscale 4, **5960 (2012)** Impact Factor: 6.233

Colour degradation of artworks: an ab-initio approach of X-ray, electronic and optical spectroscopy analyses of vermilion photodarkening
C. Hogan and F. Da Pieve
J. Analitical Atomic Spectrometry 30, 588 (2015) Impact Factor 3.379

Photoelectron-Auger electron coincidence study for condensed matter,
G.Stefani, R.Gotter, A.Ruocco, F.Offi, F. Da Pieve, S.Iacobucci, A.Morgante, A.Verdini, A.Liscio, H.Yao and R.Bartynsky,
Journal of Electron Spectroscopies and Related Phenomena 141, 149 (2004) Impact Factor : 1.750

Multiple scattering approach to two-electron resonant emission from solids,
F. Da Pieve**,** S. Di Matteo, D. Sebilleau, R. Gunnella, G. Stefani and C.R. Natoli
Phys. Rev. B 78, 035122 (2008) Impact Factor: 3.718

Real space Green's function approach to angle-resolved resonant photoemission: spin polarization and circular dichroism in itinerant magnets
F. Da Pieve and P. Krüger
Phys. Rev. B 88, 115121 (2013) Impact Factor: 3.718

First-principles calculations of Angle-Resolved and Spin-resolved photoemission Spectra of Cr(110) surfaces at the 2p-3d Cr resonance,
F. Da Pieve and P. Krüger
Phys. Rev. Lett. 110, 127401 (2013) Impact Factor: 7.645

Spin-dependent on-site electron correlations and localization in itinerant ferromagnets
R. Gotter, G. Fratesi, R. A. Bartynski, F. Da Pieve, F. Offi, A. Ruocco, M. I. Trioni, G. P. Brivio, G. Stefani
Phys. Rev. Lett. 109, 126401 (2012) Impact Factor: 7.645

A Time Dependent DFT Study of the Efficiency of Polymers for Organic Photovoltaics at the Interface with PCBM
N. Van den Brande, G. Van Lier, F. Da Pieve, G. Van Assche, B. Van Mele, F. De Proft, P. Geerlings,
RSC Advances 4, **52658 (2014)** Impact Factor: 3.289

M3M45M45 Auger lineshape measured from the Cu(111) surface: Multiplet term selectivity in angle-resolved Auger-photoelectron coincidence spectroscopy,
R. Gotter, F. Da Pieve, F. Offi, A. Ruocco, A. Verdini, H. Yao, R. Bartynski, and G. Stefani,
Phys. Rev. B 79, 075108 (2009) Impact Factor: 3.718

TESI DOTTORATO

"Correlation and polarization effects in two electron resonant emission: a multiple scattering approach"

ELENCO DELLE PUBBLICAZIONI E DELLA TESI DI DOTTORATO PRESENTATE

1. **S. Iubini**, *The nonequilibrium discrete nonlinear Schrödinger equation*, Tesi di dottorato in Fisica e Astronomia, Università di Firenze, XXVI ciclo

2. **S. Iubini**, L. Chirondojan, G.-L. Oppo, A. Politi, P. Politi, *Dynamical freezing of relaxation to equilibrium*, *Physical Review Letters*, **122**, 084102 (2019)

3. **S. Iubini**, E. Orlandini, D. Michieletto, M. Baiesi, *Topological sieving of rings according to their rigidity*, *ACS Macro Letters*, **7**, 1408-1412 (2018)

4. **S. Iubini**, P. Di Cintio, S. Lepri, R. Livi, L. Casetti, Heat transport in oscillator chains with long-range interactions coupled to thermal reservoirs, *Physical Review E* (Editors' suggestion), **97** 032102 (2018)

5. S. Pouyandeh, **S. Iubini**, S. Jurinovich, Y. Omar, B. Mennucci, F. Piazza, *Exciton transport in the PE545 complex: insight from atomistic QM/MM-based quantum master equations and elastic network models*, *Physical Biology*, **14** 066001 (2017)

6. **S. Iubini**, A. Politi, P. Politi, *Relaxation and coarsening of weakly-interacting breathers in a simplified DNLS chain*, *Journal of Statistical Mechanics*, **7** 073201 (2017)

7. **S. Iubini**, S. Lepri, R. Livi, A. Politi, *Coupled transport in rotor models*, *New Journal of Physics*, **18** 083023 (2016)

8. **S. Iubini**, O. Boada, Y. Omar, F. Piazza, *Transport of quantum excitations coupled to spatially extended nonlinear many-body system*, *New Journal of Physics*, **17** 113030 (2015)

9. **S. Iubini**, S. Lepri, R. Livi, A. Politi, *Boundary-induced instabilities in coupled oscillators*, *Physical Review Letters*, **112** 134101 (2014)

10. **S. Iubini**, A. Politi, P. Politi, *Coarsening dynamics in a simplified DNLS model*, *Journal of Statistical Physics*, DOI: 10.1007/s10955-013-0896-4 (2013)

11. **S. Iubini**, S. Lepri, R. Livi, A. Politi, *Off-equilibrium Langevin dynamics of the discrete nonlinear Schrödinger chain*, *Journal of Statistical Mechanics*, P08017 (2013)

12. **S. Iubini**, R. Franzosi, R. Livi, G.-L. Oppo, and A. Politi, *Discrete breathers and negative temperature states*, *New Journal of Physics*, **15** 023032 (2013)

13. **S. Iubini**, S. Lepri, A. Politi, *Nonequilibrium discrete nonlinear Schrödinger equation*, *Physical Review E*, **86** 011108 (2012)

PUBBLICAZIONI SCIENTIFICHE SELEZIONATE AI FINI DELLA VALUTAZIONE

S. Laricchia, E. Fabiano, F. Della Sala, Frozen density embedding with hybrid functionals, *Journal of Chemical Physics* **133**, 164111 (2010);
[nome file: JCP_133_164111_2010.pdf]

Lucian A. Constantin, E. Fabiano, **S. Laricchia**, and F. Della Sala, Semiclassical Neutral Atom as a Reference System in Density Functional Theory, *Physical Review Letter* **106**, 186406 (2011);
[nome file: PRL_106_186406_2011.pdf]

S. Laricchia, E. Fabiano, Lucian A. Constantin, and F. Della Sala, Generalized Gradient Approximations of the Noninteracting Kinetic Energy from the Semiclassical Atom Theory: Rationalization of the Accuracy of the Frozen Density Embedding Theory for Nonbonded Interactions, *Journal of Chemical Theory and Computation* ***7 (8),*** *2439 (2011);*
[nome file: JCTC_7_2439_2011.pdf]

S. Laricchia, E. Fabiano, and F. Della Sala, Frozen Density Embedding Calculations with the orbital-dependent localized Hartree-Fock Kohn-Sham potential, *Chemical Physics Letter* **518**, 114-118 (2011);
[nome file: CPL_518_114_2011.pdf]

S. Laricchia, E. Fabiano, and F. Della Sala, On the accuracy of frozen density embedding calculations with hybrid and orbital-dependent functionals for non-bonded interaction energies, *Journal of Chemical Physics* **137**, 014102 (2012).
[nome file: JCP_137_014102_2012.pdf]

S. Laricchia, E. Fabiano, and F. Della Sala, Semilocal and hybrid density embedding calculations of ground-state charge-transfer complexes, *Journal of Chemical Physics* **138,** 124112 (2013).
[nome file: JCP_138_124112_2013.pdf]

S. Laricchia, NEW DEVELOPMENTS IN SUBSYSTEM FORMULATION OF DENSITY FUNCTIONAL THEORY, Tesi di Dottorato;
[nome file: PhD_thesis_laricchia-savio.pdf]

E. Fabiano, **S. Laricchia**, F. Della Sala, Frozen density embedding with non-integer subsystems' particle numbers, *Journal of Chemical Physics* **140**, 114101 (2014);
[nome file: JCP_140_114101_2014.pdf]

S. Laricchia, L. A. Constantin, E. Fabiano, F. Della Sala, Laplacian-level kinetic energy approximations based on the fourth-order gradient expansion: global assessment and application to the subsystem formulation of Density Functional Theory, *Journal of Chemical Theory and Computation* **10 (1)**, 164 (2014);
[nome file: JCTC_10_164_2014.pdf]

S. Smiga, E. Fabiano, **S. Laricchia**, L. A. Constantin, F. Della Sala, Subsystem Density Functional Theory with meta-generalized gradient approximation exchange-correlation functionals, *Journal of Chemical Physics* **142**, 154121 (2015).
[nome file: JCP_142_154121_2015.pdf]

J. E. Bates, **S. Laricchia**, A. Ruzsinszky, Nonlocal energy-optimized kernel: Recovering second-order exchange in the homogeneous electron gas, *Physical Review B* **93**, 045119 (2016).
[nome file: PRB_93_045119_2016.pdf]

L. Chiodo, M. Salazar, A. Romero, **S. Laricchia**, F. Della Sala, and A. Rubio, Structure, electronic, and optical properties of TiO_2 atomic clusters: An ab initio study, *J. Chem. Phys.* **135**, 244704 (2011).
[nome file: JCP_135_244704_2011.pdf]

K. Chen, B. Du, R. Zhang, C. Di Paola, **S. Laricchia**, N. Bonini, C. Weber, I. Abrahams, H. Yan, M. Reece, Enhanced thermoelectric performance of Sn-doped p-type Cu_3SbS_4, *Journal of Material Chemistry C* **6**, 8546 (2018).
[nome file: JMCC_6_8546_2018.pdf]

Elenco Pubblicazioni (limitate a 12)

1. Minder, M., Pittaluga, M., Roberts, G. L., Lucamarini, M., Dynes, J. F., Yuan, Z. L., Shields, A. J. Experimental quantum key distribution beyond the repeaterless secret key capacity, *Nature Photonics* 13, pp. 334-338 (2019). DOI: 10.1038/s41566-019-0377-7.
2. Lucamarini, M., Yuan, Z.L., Dynes, J.F., Shields, A.J. Overcoming the rate-distance limit of quantum key distribution without quantum repeaters (2018) *Nature*, 557 (7705), pp. 400-403. DOI: 10.1038/s41586-018-0066-6
3. Lucamarini, M., Ward, M. B., Yuan, Z. L., Shields, A. J. *et al.* Implementation Security of Quantum Cryptography. ETSI White Paper No. 27, ISBN No. 979-10-92620-21-4 (July 2018). https://www.etsi.org/images/files/ETSIWhitePapers/etsi_wp27_qkd_imp_sec_FINAL.pdf
4. Comandar, L.C.(*), Lucamarini, M.(*), Fröhlich, B., Dynes, J.F., Sharpe, A.W., Tam, S.W.-B., Yuan, Z.L., Penty, R.V., Shields, A.J. Quantum key distribution without detector vulnerabilities using optically seeded lasers (2016) *Nature Photonics*, 10 (5), pp. 312-315. DOI: 10.1038/nphoton.2016.50 (*)Equally first authors
5. Lucamarini, M., Choi, I., Ward, M.B., Dynes, J.F., Yuan, Z.L., Shields, A.J. Practical security bounds against the Trojan-horse attack in quantum key distribution (2015) *Physical Review X*, 5 (3), 031030. DOI: 10.1103/PhysRevX.5.031030
6. Fröhlich, B., Dynes, J.F., Lucamarini, M., Sharpe, A.W., Yuan, Z., Shields, A.J. A quantum access network (2013) *Nature*, 501 (7465), pp. 69-72. DOI: 10.1038/nature12493
7. Lucamarini, M., Patel, K.A., Dynes, J.F., Fröhlich, B., Sharpe, A.W., Dixon, A.R., Yuan, Z.L., Penty, R.V., Shields, A.J. Efficient decoy-state quantum key distribution with quantified security (2013) *Optics Express*, 21 (21), pp. 24550-24565. DOI: 10.1364/OE.21.024550
8. Yuan, Z.L., Lucamarini, M., Dynes, J.F., Fröhlich, B., Plews, A., Shields, A.J. Robust random number generation using steady-state emission of gain-switched laser diodes (2014) *Applied Physics Letters*, 104 (26), art. no. 261112. DOI: 10.1063/1.4886761
9. Lucamarini, M., Vallone, G., Gianani, I., Mataloni, P., Di Giuseppe, G. Device-independent entanglement-based Bennett 1992 protocol (2012) *Physical Review A* 86 (3), 032325. DOI: 10.1103/PhysRevA.86.032325
10. Lucamarini, M., Kumar, R., Di Giuseppe, G., Vitali, D., Tombesi, P. Compensating the noise of a communication channel via asymmetric encoding of quantum information (2010) *Physical Review Letters*, 105 (14), 140504. DOI: 10.1103/PhysRevLett.105.140504
11. Lucamarini, M., Paganelli, S., Mancini, S. Two-qubit entanglement dynamics in a symmetry-broken environment (2004) *Physical Review A* 69 (6), 062308, pp. 062308. DOI: 10.1103/PhysRevA.69.062308
12. Lucamarini, M., Mancini, S. Secure deterministic communication without entanglement (2005), *Physical Review Letters*, 94 (14), art. no. 140501. DOI: 10.1103/PhysRevLett.94.140501

Tesi di dottorato

Tesi di Dottorato di Ricerca in Fisica "Quantum Decoherence and Quantum Cryptography" (teorica), con Prof. F. De Pasquale (Univ. di Roma "Sapienza") e Prof. S. Mancini (Univ. di Camerino). Data: 18 febbraio 2005. Giudizio: Ottimo.

1. M. Müller, S. Stankic , O. Diwald, E. Knözinger , P.V. Sushko , P.E. Trevisanutto, and A.L. Shluger , *Effect of protons on the optical properties of oxide nanostructures*, J. Am. Chem. Soc. 129(41):12491, 2007.
2. P.E. Trevisanutto, C. Giorgetti, L. Reining, M. Ladisa, V. Olevano, *Ab initio dynamical correlation effects in graphene: disentangling kinks* , Phys. Rev. Lett. 101, 226405 (2008) .
3. P. E. Trevisanutto, M. Holzmann, M. Côté., V. Olevano *High-energy excitonic effects in graphite and graphene:* also in cond. Mat arXiv: 0909.1682. Phys. Rev. B 81, 121405(R) (2010).
4. T. Rangel, A. Ferretti, P. E. Trevisanutto, V. Olevano, G.-M. Rignanese. *Transport properties of molecular junctions from many-body perturbation theory* ArXiv 1102.1880. Phys. Rev. B 84, 045426 (2011).
5. T. Rangel, D. Kecik, P. E. Trevisanutto, G.-M. Rignanese, H. Van Swygenhoven, and V. Olevano. *Band structure of gold from many-body perturbation theory.* Phys. Rev. B **86**, 125125 (2012). also in arXiv: 1203.4508v1
6. P. E. Trevisanutto, A. Terentjevs, L. A. Constantin, V. Olevano, and F. Della Sala. Optical spectra of solids obtained by time-dependent density-functional theory with Jellium with Gap Model exchange-correlation kernel. Phys. Rev. B **87**, 205143 (2013). also in in arXiv: 1210.7149
7. E. Fabiano, P. E. Trevisanutto, A. Terentjevs, L. A. Constantin, Generalized gradient approximation correlation energy functionals based on the uniform electron gas with gap model. J. Chem. Theory and Computation 10 (5), 2016 (2014)
8. A. Ziletti, A. Carvalho, P.E. Trevisanutto, D.K. Campbell, D.F. Coker, and A.H. Castro Neto. *Phosphorene oxides: bandgap engineering of phosphorene by oxidation*. Phys. Rev. B. 91, 0850407 (2015) Also in ArXiv:1410.3906v1
9. P.E. Trevisanutto and M. Millettari. *Hedin Equations in resonant Microcavities.* Phys. Rev. B 92 (23), 235303 (2015)
10. P.E. Trevisanutto and G. Vignale. *Ab initio electronic structure of quasi two-dimensional materials: a ``native" gaussian--plane wave approach.* The Journal of chemical physics 144 (20), 204122 (2016)
11. L.C. Gomes, P.E. Trevisanutto, A. Carvalho, A.S. Rodin, A.H. Castro-Neto. Strongly bound Mott-Wannier Excitons in GeS and GeSe monolayers. arXiv preprint arXiv:1607.07564. Phys. Rev. B 94 (15), 155428 (2016)
12. Teguh Citra Asmara, Yongliang Zhao, Muhammad Aziz Majidi, Christopher T. Nelson, Mary C. Scott, Yao Cai, Dongyang Wan, Daniel Schmidt, Ming Yang, Paolo E. Trevisanutto, Mallikarjuna R. Motapothula, Mark B.H. Breese, Matthew Sherburne, Mark Asta, Andrew Minor, T. Venkatesan, Andrivo Rusydi. *Tunable and low-loss correlated plasmons in Mott-like insulating oxides. Nature communications 8, 15271 (2017)*
13. *Ph.D. Thesis: Theoretical models of Photo-induced processes at surfaces of Oxides*

ELENCO PUBBLICAZIONI – ALESSIO TROIANI

1. Shaken dynamics for the 2d ising model, arXiv:1904.06257 (with V. Apollonio, R. D'Autilia, B. Scoppola and E. Scoppola)
2. Gaussian Mean Fields Lattice gas, *Journal of Statistical Physics* (2018), 170:1161, https://doi.org/10.1007/s10955-018-1984-2, (with B. Scoppola)
3. The blockage problem, *Bulletin of the Institute of Mathematics Academia Sinica (New Series)*, 8(1), 49–72, 2013, ISSN: 2304-7895 [online] (with O. Costin, J. L. Lebowitz and E. R. Speer).
4. Metastability for Kawasaki dynamics with two types of particles, PhD Thesis, 2012, ISBN 9789461914644, handle: http://hdl.handle.net/1887/20065
5. Metastability for Kawasaki dynamics with two types of particles: critical droplets, *Journal of Statistical Physics*, 149, 1013–1057, 2012, https://doi.org/10.1007/s10955-012-0637-0 (with F. den Hollander and F. R. Nardi).
6. Metastability for Kawasaki dynamics with two types of particles: stable/metastable configurations and communication heights, *Journal of Statistical Physics*, 145, 1423–1457, 2011, https://doi.org/10.1007/s10955-011-0370-0 (with F. den Hollander and F. R. Nardi).
7. Metastability for Kawasaki dynamics at low temperature with two types of particles, *Electronic Journal of Probability*, 17(2), 1–26, 2012, doi:10.1214/EJP.v17-1693 (with F. den Hollander and F. R. Nardi).

GAIA CAMISASCA, Ph.D.

PERSONAL INFORMATION

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Department of Physics, Stockholm University

Links https://orcid.org/0000-0002-0789-2641

Scopus Author ID: 55515716800

ResearchGate

EDUCATION AND WORK EXPERIENCE

Mar 2017–Present "Stockholm University"

Postdoc

Theoretical simulations to study dynamics and thermodynamics of supercooled water. Integration of user-defined analysis tools in GROMACS (C, C++). Advisor: Prof. Lars G.M. Pettersson

Nov 2013-Feb 2017 "Università degli Studi Roma Tre"

PhD in Physics

PhD in Physics at the Department of Mathematics and Physics of the university "Università degli Studi Roma Tre". PhD research project in *Cryopreservation and dynamics of supercooled water solutions*. Supervisor: Prof. Paola Gallo

Mar-Sept 2013 "Elettra Sincrotrone Trieste"

Collaborator IUVS BL

Visible and UV Raman spectroscopies, visible and UV Brillouin on liquids. Development of data analysis programs. Technical Beamline Support.

Jan 2009–Dec 2012 "Sapienza Università di Roma"

Master's Degree in Physics

Final Grade: 110/110 cum laude
Curriculum: Condensed Matter Physics, Statistical Mechanics, Phase transitions and Critical phenomena, Liquids
Master's Thesis title: *High resolution Raman spectroscopy on acetamide-water solutions*. Thesis project performed at the Elettra Sincrotrone Trieste, IUVS BL EIS Group.
Supervisors: Prof. Giancarlo Ruocco (Sapienza), Dr. Francesco D'amico (Elettra) and Dr. Claudio Masciovecchio (Elettra)

Ott 2006-Nov 2009 "Sapienza Università di Roma"

Bachelor's Degree in Physics

Final Grade: 110/110 cum laude

TEACHING ACTIVITIES

2014-2017 — Condensed Matter Physics

Teaching Assistant — Master course of Prof. Paola Gallo at Roma Tre University, Math. and Phys. Dept.

COMPUTER SKILLS

Software — GROMACS, i-PI, Lammps, MATLAB, VMD, GIMP

MD Simulations — Bio-systems: Proteins, disaccharides and organic molecules in water. Glass forming solutions of electrolytes. Water in supercooled regime and around biomolecules. Confined water in silica matrix.

Programming — C, python (Numpy/Pandas/Matplotlib/SciPy/MDAnalysis/HDF5/Jupyter Notebooks), Fortran, C++,MPI, OpenMP, Shell Script, LaTeX

Operating Systems — Linux, OSX, Microsoft Windows

HPC platforms — - Swedish National Infrastructure for Computing: Kebnekaise-HPC2N (602 nodes, 19288 cores), Abisko-HPC2N (332 nodes,15264 cores), Beskow-PDC (2060 nodes, 67456 cores), Tetralith-NSC (1892 nodes, 60544 cores);
- Classe, Stockholm University Chemical Physics Cluster (6 nodes, 192 cores);
- Roma Tre Cluster (59 nodes, 1828 cores).

HPC job queue management — PBS Torque, Slurm

LANGUAGES

Italian — Mother tongue

English — Proficient

Swedish — Beginner

COURSES & SCHOOLS IN COMPUTER SCIENCE

13-21 Jul 2014 — CCP5 Summer School *Methods in Molecular Simulations*. Held at Manchester University.

14-15 May 2015 — Course *Parallel IO and management of large scientific data*. Held at CINECA, Rome.

23-25 Feb 2015 — Course *Introduction to Parallel Computing with MPI and OpenMP*. Held at CINECA, Rome.

5-7 Feb 2016 — Course *High Performance Molecular Dynamics*. Held at CINECA, Rome.

29 Nov-1 Dec 2017 — BioExcel training course *Hands-on Introduction to HPC for Life Scientists @ EPCC*. Held at EPCC, Edinburgh.

25-29 Jun 2018 — CECAM School *Path Integral Quantum Mechanics: From the Basics to the Latest Developments*. Held

at EPFL, Lausanne.

25-26 Oct 2018 PDC-PRACE training workshop: *HPC tools for the modern era*. Held at PDC, Stockholm.

WORKSHOPS, CONFERENCES & SCHOOLS IN PHYSICS

18-22 Mar 2012 XIII International Workshop on Complex Systems. Held at Andalo, Italy. Poster Presented.

17-18 Sept 2014 Workshop *Italian Soft Days*. Held at Sapienza Università di Roma, Rome.

10-12 Jun 2015 Workshop *Roma Tre Workshop on Water under Extreme Conditions*. Held at Università degli Studi Roma Tre, Rome. Oral Presentation.

7-12 Sept 2015 Conference *Frontiers in Water Biophysics*. Held at Ettore Majorana Foundation and Center for Scientific Culture in Erice, Italy. Poster Presented.

30 Nov-5 Dec 2015 Conference *MRS Fall Meeting and Exhibit 2015, Symposium Liquids and Glassy Soft Matter-Theoretical and Neutron Scattering Studies*. Held in Boston, USA. Poster Presented.

6-10 Jun 2016 Conference *Sitges Conference on Statistical Mechanics: "Nonequilibrium Phenomena in Con- fined Systems"*. Held in Barcelona, Spain. Oral Presentation.

23-26 Jul 2016 Conference *STAT-PHYS 2016 satellite meeting: Water X: exotic properties of water under extreme conditions*. Held in Nice, France. Poster Presented.

8-9 Jun 2017 CoT$_X$S Mini-Workshop. Held at Stockholm University, Stockholm. Poster Presented.

14-16 Jun 2017 Workshop *Roma Tre Congress on Water under Extreme Conditions*. Held at Università degli Studi Roma Tre, Rome. Posters Presented.

25-26 Sept 2017 CoT$_X$S Mini-Workshop. Held at Stockholm University, Stockholm.

4-1 Jul 2018 International School of Water and Water System, *Water and the water systems - The hydrophobic effect*. Held at Ettore Majorana Foundation and Center for Scientific Culture in Erice, Italy. Poster Presented & Oral Presentation.

22-27 Jul 2018 Gordon Research Conference *Water and Aqueous Solutions*. Held at Holderness, NH USA. Poster Presented.

ORGANIZATION OF MEETINGS

10-12 Jun 2015 Local organizing committee "Roma Tre Workshop on Water under Extreme Conditions", Università degli Studi Roma Tre, Rome.

14-16 Jun 2017 Local organizing committee "Roma Tre Congress on Water under Extreme Conditions", Università degli Studi Roma Tre, Rome.

12-14 Jun 2019 Local organizing committee "Roma Tre Congress on Water under Extreme Conditions", Università degli Studi Roma Tre, Rome.

AWARDS

2015 Travel grant, Ettore Majorana Foundation. I used the grant to participate to the conference Frontiers in Water Biophysics.

2017 BioExcel travel grant. I used the grant to participate to the EPCC training course.

2018 Scholarship, Royal Swedish Academy of Sciences. I used the grant to participate to the CECAM school on Path Integrals.

2018 Travel grant, Wenner-Gren Foundation. I used the grant to participate to the Gordon Research Conference on water.

2018 Travel grant, Ettore Majorana Foundation. I used the grant to participate to the Erice school on Water and water systems.

REFERENCES

Lars Pettersson, Prof.
Postdoc advisor
Department of Physics, Stockholm University
Phone: +46-070-495 1990, Email: lgm@fysik.su.se

Paola Gallo, Prof.
PhD supervisor
Department of Physics, Roma Tre University
Phone: +39-06-5733 7310, Email: gallop@fis.uniroma3.it

Fivos Perakis, Prof.
Collaborator
Department of Physics, Stockholm University
Phone: +46-076-426 8813, Email: f.perakis@fysik.su.se

Mauro Rovere, Prof.
PhD Collaborator
Department of Physics, Roma Tre University
Phone: +39-06-5733 7043, Email: rovere@fis.uniroma3.it

April 23, 2019

CURRICULUM VITAE

Federico Carollo

Current professional situation

Employing entity: University of Nottingham **Type of entity:** University

Department: School of Physics and Astronomy

Professional category: Post-Doctoral Research Fellow

City employing entity: Nottingham, United Kingdom

Start date: 03/10/2016

Type of contract: Temporary employment contract **Dedication regime:** Full time

Previous positions and activities

***Employing* Entity**	**Professional category**	**Start date**
University of Trieste	Ph.D. Student	01/01/2013

Employing entity: University of Trieste **Type of entity:** University

Department: Department of Physics

City employing entity: Trieste, Friuli- Venezia Giulia, Italy

Professional category: Ph.D. Student

Start- End date: 01/01/2013 – 21/04/2016 **Duration:** 3 years – 3 months -21 days

Type of contract: Ph. D. Fellowship

Dedication regime: Full time

Education

University education

1. **University degree:** Higher degree
   Name of qualification: Bachelor Degree in Physics
   City degree awarding entity: Trieste, Friuli- Venezia Giulia, Italy
   Degree awarding entity: University of Trieste **Type of entity:** University
   Date of qualification: 21/09/2012
   Foreign qualification: Laurea Triennale in Fisica
   Final grade: 110/ 110 cum laude

2. **University degree:** Higher degree
   Name of qualification: Master Degree in Naval Architecture and Marine Engineering
   City degree awarding entity: Genova, Liguria, Italy
   Degree awarding entity: University of Genova **Type of entity:** University
   Date of qualification: 16/07/2010
   Foreign qualification: Laurea Specialistica in Ingenieria Navale
   Final grade: 110/ 110 cum laude

3. **University degree:** Higher degree
   Name of qualification: Bachelor Degree in Naval Architecture and Marine Engineering
   City degree awarding entity: Genova, Liguria, Italy
   Degree awarding entity: University of Genova **Type of entity:** University
   Date of qualification: 19/12/2007
   Foreign qualification: Laurea Triennale in Ingenieria Navale
   Final grade: 108/ 110

Doctorates

Doctorate programme: Doctorate in Theoretical Physics
Degree awarding entity: University of Trieste **Type of entity:** University
Date of degree: 21/04/2016
Thesis title: Quantum fluctuations and entanglement in mesoscopic system
Thesis director: Prof. Fabio Benatti

Language skills

Language	Listening skills	Reading skills	Spoken interaction	Speaking skills	Writing skills
English	C1	C1	C1	C1	C1
French	B2	B2	B2	B2	B2

Teaching experience

Supervision of Students

1. **Description of the activity:** Co- Supervisor of Master Degree Thesis in Physics
   Student: Jacopo Surace
   Title: Entangling two harmonic chains through a common bath
   Organising entity: University of Trieste **Type of entity:** University
   End date: 2015

2. **Description of the activity:** Informally Co- Supervising the research work of a Ph. D. student
   Student: Loredana M. Vasiloiu
   Organising entity: University of Nottingham **Type of entity:** University
   Date: 2017/ 2019

Scientific and technological experience

1. **Name of the project:** Dynamic Nuclear Polarisation And Non-Equilibrium Physics. EPSRC Grant no. EP/N03404X/1
   Degree of contribution: Researcher
   Entity where project took place: University of Nottingham **Type of entity:** University
   City of entity: Nottingham, Nottinghamshire, United Kingdom
   Funding entity or bodies: Engineering and Physical Sciences Research Council
   Start- End date: 03/10/2018 –
   Dedication regime: Full time

2. **Name of the project:** Exploring Strongly Correlated Quantum Matter with Cold Excited Atoms. FP/2007-2013/ERC Grant Agreement No. 335266 (ESCQUMA)
   Degree of contribution: Researcher
   Entity where project took place: University of Nottingham **Type of entity:** University
   City of entity: Nottingham, Nottinghamshire, United Kingdom
   Funding entity or bodies: European Research Council
   Start- End date: 03/10/2017 – 02/10/2018
   Dedication regime: Full time

3. **Name of the project:** Rydberg Soft Matter. EPSRC Grant No. EP/M014266/1
   Degree of contribution: Researcher
   Entity where project took place: University of Nottingham **Type of entity:** University
   City of entity: Nottingham, Nottinghamshire, United Kingdom
   Funding entity or bodies: Engineering and Physical Sciences Research Council
   Start- End date: 03/10/2016 – 02/10/2017
   Dedication regime: Full time

4. **Name of the project:** Fisica teorica e sperimentale sui temi dell'INFN
   Degree of contribution: Researcher
   Entity where project took place: Department of Physics **Type of entity:** University
   City of entity: Trieste, Italy
   Funding entity or bodies: Istituto Nazionale di Fisica Nucleare
   Type of entity: Public Researcher Body
   Start- End date: 01/01/2013 – 31/12/2015
   Dedication regime: Full time

Scientific and technological activities

Scientific production

Pre-prints

1. **Authors:** Federico Carollo, Edward Gillman, Hendrik Weimer, and Igor Lesanovsky
   Title: Quantum contact process
   Journal: submitted to Phys. Rev. Lett. - pre print arXiv:1902.04515 (2019)
   Available on-line at: https://arxiv.org/abs/1902.04515

2. **Authors:** Loredana M. Vasiloiu, Federico Carollo, Matteo Marcuzzi, and Juan P. Garrahan
   Title: Strong zero modes in a class of generalised Ising spin ladders with plaquette interactions
   Journal: submitted to Phys. Rev. B - pre print arXiv:1901.10211 (2019)
   Available on-line at: https://arxiv.org/abs/1901.10211

Publications

1. **Authors:** Federico Carollo, Robert L. Jack, and Juan P. Garrahan
   Title: Unraveling the large deviation statistics of Markovian open quantum systems
   Journal: PHYSICAL REVIEW LETTERS, **122** – 130605 (2019), American Physical Society
   Available on-line at: 10.1103/PhysRevLett.122.130605

2. **Authors:** Filippo M. Gambetta, Federico Carollo, Matteo Marcuzzi, Juan P. Garrahan, and Igor Lesanovsky
   Title: Discrete time crystals in the absence of manifest symmetries or disorder in open quantum systems
   Journal: PHYSICAL REVIEW LETTERS, **122** – 015701 (2019), American Physical Society
   Available on-line at: 10.1103/PhysRevLett.122.015701

3. **Authors:** Federico Carollo, Juan P. Garrahan, and Igor Lesanovsky
   Title: Current fluctuations in boundary-driven quantum spin chains
   Journal: PHYSICAL REVIEW B, **98** – 094301 (2018), American Physical Society
   Available on-line at: http://doi.org/10.1103/PhysRevB.98.094301

4. **Authors:** Carlos Pérez-Espigares, Federico Carollo, Juan P. Garrahan and Pablo I. Hurtado

   Title: Dynamical criticality in open system: non-perturbative physics, microscopic origin and direct observation

   Journal: PHYSICAL REVIEW E (Rapid), **98** – 060102 (2018), American Physical Society

   Available on-line at: http://doi.org/10.1103/PhysRevE.98.060102

5. **Authors:** Loredana M. Vasiloiu, Federico Carollo, and Juan P. Garrahan

   Title: Enhancing correlation times for edge spins through dissipation

   Journal: PHYSICAL REVIEW B, **98** – 094308 (2018), American Physical Society

   Available on-line at: http://doi.org/10.1103/PhysRevB.98.094308

6. **Authors:** Federico Carollo, Juan P. Garrahan, Igor Lesanovsky, and Carlos Pérez-Espigares

   Title: Making rare events typical in Markovian open quantum systems

   Journal: PHYSICAL REVIEW A (Rapid), **98** – 010103 (2018), American Physical Society

   Available on-line at: http://doi.org/10.1103/PhysRevA.98.010103

7. **Authors:** Fabio Benatti, Federico Carollo, Roberto Floreanini, and Heide Narnhofer

   Title: Quantum spin chain dissipative mean-field dynamics

   Journal: JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL **51**, 325001 (2018), IOP Publishing

   Available on-line at: http://doi.org/10.1088/1751-8121/aacbdb

8. **Authors:** Federico Carollo, Juan P. Garrahan, Igor Lesanovsky, and Carlos Pérez-Espigares

   Title: Fluctuating hydrodynamics, current fluctuations, and hyperuniformity in boundary-driven open quantum chains

   Journal: PHYSICAL REVIEW E, **96** – 052118 (2017), American Physical Society

   Available on-line at: http://doi.org/10.1103/PhysRevE.96.052118

9. **Authors:** Fabio Benatti, Federico Carollo, Roberto Floreanini, and Heide Narnhofer

   Title: Quantum fluctuations in mesoscopic systems

   Journal: JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL **50**, 423001 (2017), IOP Publishing

   Available on-line at: http://doi.org/10.1088/1751-8121/aa84d2

10. **Authors:** Fabio Benatti, Federico Carollo, and Roberto Floreanini

    Title: Dissipative entanglement of quantum spin fluctuations

    Journal: JOURNAL OF MATHEMATICAL PHYSICS **57**, 062208 (2016), AIP Publishing

    Available on-line at: http://doi.org/10.1063/1.4954072

11. **Authors:** Fabio Benatti, Federico Carollo, Roberto Floreanini, and Jacopo Surace

    Title: Long-lived mesoscopic entanglement between two damped infinite harmonic chains

    Journal: JOURNAL OF STATISTICAL PHYSICS **168**, pp 620- 651 (2016), Springer

    Available on-line at: 10.1007/s10955-017-1817-8

12. **Authors:** Fabio Benatti, Federico Carollo, Roberto Floreanini, and Heide Narnhofer

    Title: Non-Markovian mesoscopic dissipative dynamics of open quantum spin chains

Journal: PHYSICS LETTERS A, **380** – pp. 381- 389 (2016), Elsevier

Available on-line at: http://doi.org/10.1016/j.physleta.2015.10.062

13. **Authors:** Fabio Benatti, Federico Carollo, and Roberto Floreanini

    Title: Dissipative dynamics of quantum fluctuations

    Journal: ANNALEN DER PHYSIK **527**, pp 639- 655 (2015), Wiley

    Available on-line at: http://doi.org/10.1002/andp.201500165

14. **Authors:** Fabio Benatti, Federico Carollo, and Roberto Floreanini

    Title: Environment induced entanglement in many-body mesoscopic systems

    Journal: PHYSICS LETTERS A, **378** – pp. 1700- 1703 (2014), Elsevier

    Available on-line at: http://doi.org/10.1016/j.physleta.2014.04.034

15. **Authors:** Fabio Benatti, and Federico Carollo

    Title: A non-Markovian dissipative Maryland model

    Journal: OPEN SYSTEMS & INFORMATION DYNAMICS **20**, 1340001 (2013), World Scientific

    Available on-line at: http://doi.org/10.1142/S1230161213400015

16. **Authors:** Giovanni B. Benvenuto, Daniele Bertetta, Ugo Campora, and Federico Carollo

    Title: Dynamic simulation of a COGAS ship propulsion plant

    Journal: RESPONSE OF SHIPS AND SHIPPING RESEARCH TO THE INTERNATIONAL CRISIS. Proceeding of the 17th International Conference on Ships and Shipping Research (NAV 2012), Napoli, 17-19 October 2012

    ISBN: 9788890439421

17. **Authors:** Giovanni B. Benvenuto, Daniele Bertetta, Ugo Campora, and Federico Carollo

    Title: COGAS plant as possible future alternative to the diesel engine for the propulsion of large ships

    Journal: SUSTAINABLE MARITIME TRANSPORTATION AND EXPLOITATION OF SEA RESOURCES. Rizzuto & Guedes Soares (eds) Proceeding of the 14th International Conference on Maritime Association of Mediterranean (IMAM 2011), Genova, 13-16 September 2011. London: Taylor & Francis Group pp 603- 614 CRC Press, 2011

Works submitted to national or international conferences

1. **Title of the work:** Current fluctuations in boundary-driven quantum spin chains

   Name of the conference: Transport in strongly correlated quantum systems

   Type of event: Conference

   Type of participation: Invited talk

   City of event: Natal, Brazil

   Date of event: 16/07/2018

   End date: 03/08/2018

   Organising entity: International Institute of Physics

   Type of entity: University Research Institute

   City organising entity: Natal, Brazil

   Available on-line at: <https://www.iip.ufrn.br/eventsdetail.php?inf===QTU1Ue>

2. **Title of the work:** Current fluctuations in boundary-driven quantum spin chains
   Name of the conference: Conference on Non-Equilibrium Systems “CONES 2018”
   Type of event: Conference
   Type of participation: Talk
   City of event: London, United Kingdom
   Date of event: 25/06/2018
   End date: 27/06/2018
   Organising entity: King's College London
   Type of entity: University
   City organising entity: London, United Kingdom
   Available on-line at: <https://cnes.kcl.ac.uk/cones-2018/#>

3. **Title of the work:** Current fluctuations in boundary-driven quantum spin chains
   Name of the conference: Seminar @ DF- TS
   Type of event: Seminar
   Type of participation: Talk
   City of event: Trieste, Friuli Venezia Giulia, Italy
   Date of event: 02/03/2018
   Organising entity: Department of Physics
   Type of entity: University Department
   City organising entity: Trieste, Italy
   Available on-line at: <https://df.units.it/it/eventi/22819>

4. **Title of the work:** Environment induced collective entanglement in mesoscopic systems
   Name of the conference: Chaos and Quantum Information Seminars
   Type of event: Seminar
   Type of participation: Talk
   City of event: Krakow, Poland
   Date of event: 30/05/2016
   Organising entity: Marian Smoluchowski Institute of Physics
   Type of entity: University Department
   City organising entity: Krakow, Poland
   Available on-line at: <http://chaos.if.uj.edu.pl/ZOA/?,24&sLang=en>

5. **Title of the work:** Environment induced collective entanglement in mesoscopic systems
   Name of the conference: 605. WE- Heraeus- Seminar on Macroscopic Entanglement
   Type of event: Conference
   Type of participation: Poster
   City of event: Bad Honnef, Germany
   Date of event: 17/01/2016
   End date: 22/01/2016
   Organising entity: Max Planck Institute for the Science of Light
   Type of entity: University Research Institute

City organising entity: Erlangen, Germany

Available on-line at:

<http:www.fysik.dtu.dk/english/research/qpit/events/previous-events/we-heraeus-seminar-2016>

6. **Title of the work:** Non-Markovian many-body dynamics

   Name of the conference: Analysis, Math- Phys, and Quantum

   Type of event: Seminar

   Type of participation: Invited talk

   City of event: Trieste, Friuli Venezia Giulia, Italy

   Date of event: 05/11/2015

   Organising entity: SISSA

   Type of entity: Research Institute

   City organising entity: Trieste, Italy

   Available on-line at: <https://people.sissa.it/~alemiche/qm-seminar-2015-2016.html>

7. **Title of the work:** Non-Markovian mean-field dissipative dynamics

   Name of the conference: Cond- Math Seminars

   Type of event: Seminar

   Type of participation: Talk

   City of event: Roma, Lazio, Italy

   Date of event: 03/11/2015

   Organising entity: Roma Tre

   Type of entity: University

   City organising entity: Roma, Italy

   Available on-line at: <http://www1.mat.uniroma1.it/people/correggi/>

8. **Title of the work:** Mean-field dissipative dynamics in infinite quantum systems

   Name of the conference: 8th Italian Quantum Information Science Conference

   Type of event: Conference

   Type of participation: Talk

   City of event: Monopoli, Puglia, Italy

   Date of event: 10/09/2015

   End date: 12/09/2015

   Organising entity: Dipartimento Interateneo di Fisica

   Type of entity: University Department

   City organising entity: Bari, Puglia, Italy

   Available on-line at: <https://agenda.infn.it/conferenceDisplay.py?confId=9324>

9. **Title of the work:** Quantum fluctuations and mesoscopic dissipative dynamics

   Name of the conference: 51 Winter School of Theoretical Physics “Irreversible dynamics: nonlinear, nonlocal and non-Markovian manifestation

   Type of event: Conference

   Type of participation: Lecturer

   City of event: Ladek Zdroj, Poland

Date of event: 09/02/2015

End date: 14/02/2015

Organising entity: Institut of Theoretical Physics

Type of entity: University Department

City organising entity: Wroclaw, Poland

Available on-line at: <http://ift.uni.wroc.pl//~karp51/>

10. **Title of the work:** Environment induced entanglement in mesoscopic system

    Name of the conference: Mini- Symposium “On Entanglement”

    Type of event: Seminar

    Type of participation: Talk

    City of event: Vienna, Austria

    Date of event: 10/12/2014

    Organising entity: Faculty of Physics, University of Vienna

    Type of entity: University Department

    City organising entity: Vienna, Austria

    Available on-line at: <https://physik-newsarchiv.univie.ac.at/fileadmin/user_upload/f_physik/Vortraege/GP-MP-TP/FedericoCarollo_10.12.14.pdf/>

11. **Title of the work:** Environment induced entanglement in mesoscopic system

    Name of the conference: Quantum Roundabout

    Type of event: Conference

    Type of participation: Talk

    City of event: Nottingham, Nottinghamshire, United Kingdom

    Date of event: 29/06/2014

    End date: 02/07/2014

    Organising entity: School of Mathematical Science

    Type of entity:

    City organising entity: Nottingham, United Kingdom

    Available on-line at: <http://paft14.sa.infn.it/programma.html>

12. **Title of the work:** COGAS plant as possible future alternative to the diesel engine for the propulsion

    Name of the conference: IMAM 2011 XIV Congress of the International Maritime Association of the Mediterranean

    Type of event: Conference

    Type of participation: Talk

    City of event: Genova, Liguria, Italy

    Date of event: 12/09/2011

    End date: 16/09/2011

    Organising entity: Interactional Maritime Association

    Type of entity: Associations and Groups of the Mediterranean

    Available on-line at: <http://www.imamhomepage.org/conferences,aspx>

Other achievements

Stays in public or private R&D centres

Entity: Erwin Schrödinger International Institute for Mathematics and Physics (ESI)

City of entity: Vienna, Austria

Start- End date: 07/06/2015 – 20/06/2015

Obtained grants and scholarships

1. **Name of the grant:** Research Fellow Contract

   Aims: Post-Doctoral

   Awarding entity: University of Nottingham

   Type of entity: University

   Conferral date: 03/10/2016

   Entity where activity was carried out: University of Nottingham

   Faculty, institute or centre: School of Physics and Astronomy

2. **Name of the grant:** Fisica teorica e sperimentale sui temi dell'INFN (Theoretical and experimental physics on thematics of the INFN)

   Awarding entity: Istituto Nazionale di Fisica Nucleare

   Type of entity: Public Research Body

   Conferral date: 01/01/2013 **Duration:** 3 years

   End date: 31/12/2015

   Entity where activity was carried out: University of Trieste

   Faculty, institute or centre: Department of Physics

3. **Name of the grant:** Scholarship Pretto- Cassanello Foundation Academic Year 2008/2009

   City awarding entity: Genova, Liguria, Italy

   Awarding entity: Fondazione Pretto- Cassanello

   Amount of the grant: 2500 €

   Type of entity: Foundation

   Conferral date: 2010

   Entity where activity was carried out: University

Scientific societies and professional association

Name of the society: Istituto Nazionale di Fisica Nucleare (INFN)

City affiliation entity: Trieste, Friuli Venezia Giulia, Italy

Start- End date: 01/01/2013 – 21/04/2016

Name of the society: Centre for the Mathematics and Theoretical Physics of Quantum Non- Equilibrium Systems (CQNE)

City affiliation entity: Nottingham, Nottinghamshire, United Kingdom

Start- End date: 03/10/2016

CURRENT POSITION

Research Scientist (fixed-term contract), leader of the H2020 ESC2RAD project www.esc2rad.eu
Belgian Institute for Space Aeronomy (BIRA-IASB), Brussels (BE)
My expertise is mainly in theoretical/computational materials science and in the study of fundamental problems in spectroscopy in chemical-physics/condensed matter; recently, I started an activity on the study of ion impact in solar cells, 2D materials with high radiation tolerance and biological matter, of importance in the context of space and planetary missions

WORK EXPERIENCE

03/2018-Present

Research scientist, Scientific Coordinator of the H2020 ESC2RAD project

Royal Belgian Institute for Space Aeronomy, Brussels, Belgium, www.bira-iasb.be

- Research activity in the context of the H2020 project ESC2RAD www.esc2rad.eu , focussed on radiobiological damage and instrumental degradation due to radiation in different Space weather conditions in future human deep space missions and missions to Mars; Management, Reporting, Coordination of the consortium's activity, Organization of events (workshops, outreach activities ...)

Sector Research

03/2016-02/2018

Scientific Assistant, Management of national and ESA's projects

Royal Belgian Institute for Space Aeronomy, Brussels, Belgium, www.bira-iasb.be

- Management, reporting and dissemination activities related to the ESA's SPENVIS project (www.spenvis.oma.be, for reliable estimation of radiation effects on astronauts and instruments on board of spacecraft) and to the Space Weather Coordination Centre in the context of the Space Situation Awareness (SSA) programme (http://swe.ssa.esa.int/).
- Providing science-based reports for influencing ESA strategy
- Management of the communication flow between different expert groups in Europe linked to the SSA programme in case of severe Space weather events and consequent impacts on the ISS, on satellites, power grids, aviation, …

Sector Management, of Research Projects

05/2014-02/2016

Marie Curie Fellow (IEF)

École Polytechnique de Palaiseau, Palaiseau, France

- Research in the field of light-matter interaction, on both gaseous targets (molecules and atoms) and materials, for both fundamental scientific aims and nanotechnology applications;

Sector Research, Teaching, Supervision of PhD and Master students

11/2013-04/2014

Visiting Scientist
Université libre de Bruxelles (ULB), Brussels, Belgium

- Research in the field of light-matter interaction, on both gaseous targets (molecules and atoms) and materials, for *environmental pollutions induced by heavy metals* and *nanotechnology applications*

Sector Research

10/2012-10/2013

Postdoctoral Researcher
Free Universiteit Brussel (VUB), Brussels, Belgium

- Research in the field of light-matter interaction, on both gaseous targets (molecules and atoms) and materials, for *environmental pollutions induced by heavy metals* and scientific problems in *astronomy*

Sector Research, Teaching, Supervision of PhD and Master students

01/2012-09/2012

Postdoctoral Researcher
University Antwerp (UA), Antwerp, Belgium

- Research in the field of light-matter interaction, on both gaseous targets (molecules and atoms) and materials, for *cultural heritage applications*

Sector Research, Teaching, Supervision of PhD and Master students

09/2011-01/2012

IT Expert in Secure Communications
Italian Minister of Foreign Affairs and International Cooperation, Roma, Italy

- Managing the IT cryptographic systems to secure the communications between the Minister, the EU and Italian ambassades; performing the first tests on the systems that would have been then used by the Galileo satellite, together with the base at Fucino (IT), in case of defense scenarios
- Reporting results of tests to several government members and members of the Italian Minister of Defense

Sector IT, cryptography, management

09/2010-09/2011

Postdoctoral Researcher
University Antwerp (UA), Antwerp, Belgium

- Research in the field of light-matter interaction, on both gaseous targets (molecules and atoms) and materials, for *cultural heritage* applications

Sector Research, Teaching, Supervision of PhD and Master students

09/2008-09/2010

Postdoctoral Researcher
Catholic University of Louvain La Neuve (UCL), Louvain La Neuve, Belgium

- Research in the field of light-matter interaction, on both gaseous targets (molecules and atoms) and materials, for *solar cells applications*

Sector Research, Teaching, Supervision of PhD and Master students

03/2007-09/2008

Postdoctoral Researcher
Universite de Bourgogne, Dijon, France

- Research in the field of light-matter interaction, on both gaseous targets (molecules and atoms) and materials, for *solar cells applications*

Sector Research, Teaching, Supervision of PhD and Master students

2/11/2006-31/01/2007

Short Collaboration contract
University Roma Tre, Rome, Italy

- Research in the field of light-matter interaction, on both gaseous targets (molecules and atoms)

CAREER BREAKS FROM RESEARCH

14/10/2014-16/04/2015	Maternity leave followed by illness
19/08/2016-01/12/2016	Maternity leave
01/03/2016-28/02/2018	Management of European Space Agency's projects

EDUCATION AND TRAINING

11/2003-02/2007

PhD in Physics

University Roma Tre, Rome, Italy, with internal supervisor Prof. G. Stefani (University Roma Tre, Italy) and external supervisor Dr. C.R. Natoli at the National Institute for Nuclear Physics (INFN, Frascati, Italy)

Title of the thesis: Correlation and polarization effects in two-electron resonant emission: a multiple scattering approach

10/1998-07/2003

Master in Physics – 110/110 cum Laude

University Roma Tre, Rome, Italy

09/1993-07/1998

Diploma Secondary High School – 60/60

Secondary High School "Primo Levi", Rome, Italy (scientific orientation)

Schools/Courses in theory and computation in condensed matter/chemical-physics

"School on Dynamical Mean Field Theory – LMTO", associated to the workshop "Recent progress in Dynamical Mean-Field Theory and GW calculations", 17-20th December 2012, Strasbourg (France)
"Time Dependent Density Functional Theory" 1th-10th September 2008, Benasque (Spain)
"From synchrotron to FEL radiation: new opportunities for science in Frascati", &!-20th June 2007, Rome (Italy)
"National School for Synchrotron Radiation", 10-21st October 2005, Frascati, Rome (Italy)
"Magnetism and Synchrotron Radiation", 10-15th October 2004, Mittelwihr (France)

Schools/Courses in IT: Grid, HPC, AI

"Machine Learning for Materials Science" 6-8th May 2019, Aalto University (Finland)
Course: "Linux and networking", 23rd May-1st June 2006, Rome, CITICord (Italy)
Course "Grid Technologies for system administrators and users" 18-21 April 2006, Rome, INFN Roma Tre (Italy)
Course "Grid Technologies for users and applications developers" 11-13 September 2006, Rome, INFN Roma Tre (Italy)

Knowledge of codes (materials science, chemical-physics)

ABINIT, Wien2k, VASP, OCTOPUS, YAMBO, MsSPEC, …

AWARDS/GRANTS, MEMBERSHIP, REVIEWING ACTIVITY

Awards and Competitions Wons

2015: classified first in section 1 (solid state physics, chem. phys.) of FRS-FNRS (Belgium)
2014: classified first in section 1 (solid state physics, chem. phys.) of FRS-FNRS (Belgium)
2007: I have won a competition in cryptography and secure communications, for a permanent job at the Italian Minister of Foreign Affairs (ROI team, Reti e Organizzazioni Internazionali). I arrived 1st over 756 candidates.
2009: Award Best seminar, Université Catholique de Louvain, Belgium
2006: National Award for the work: ¨Two Electron-Resonant emission in the Multiple Scattering Approach¨ received from the Italian Society for Synchrotron Radiation (SILS), Naples, 6-8th July
2005: National Award for ¨Young researchers in physics¨, in occasion of the world year of Physics, funded by the Italian Minister of Research, for ¨excellent scientific activity dealing with both theory and experiments

Grants/funding history

H2020 Research and Innovation Action (SPACE COMPET-5 –call 2017) project ESC2RAD, ID 776410; Total amount: 1300000 euro, among which 800000 euro only for my team at BIRA-IASB (the rest is shared among the partners Prof. E. Artacho, U. Cambridge and team leader at the CIC nanoGUNE centre in San Sebastian, and Prof. J. Kohanoff, Director of the atomistic simulation center at Queen's University of Belfast)
FP7: Marie Curie IEF FP7-PEOPLE-2013-IEF project RESCOR, ID 627569
CINECA: 2012: CINECA Award of 1 million CPU hours: project PHYSART
2012: Grant to participate to the DMFT-LMTO School associated to the workshop "Recent progress in Dynamical Mean-Field Theory and GW calculations"(17-20th December 2012, Strasbourg, France
2008: Grant to participate to the School "Time Dependent DFT" (1th-10th Sept 2008,Benasque, Spain)

Memberships

- Belgian Representative of the Cost Action 17126 "Towards understanding and modelling intense electronic excitations"
- Member of the European Geophysical Union (EGU)
- Member of the European Theoretical Spectroscopy Facility (ETSF)
- Member of the Belgian FNRS Contact group for Synchrotron Radiation
- Member of the European Network EUROPLANET (http://www.europlanet-2020-ri.eu/)
- Member of the Belgian FNRS Contact group for Astrobiology (http://astrobio.oma.be/)
- Member of the Psi-k society
- Member of the EUSpec COST action AMP1306 "Modern Tools for Advanced Materials" (2014-2017)
- Member of the NanoTP COST action MP0901 "Designing novel materials for nanodevices" (2010-2014)

Refereeing/Reviewing Activity

Referee for the following journals:
Phys. Rev. B, Phys. Rev. A, Phys. Rev. Lett. , Journal of Physical Chemistry C, Micron, ACS omega. Journal of Space Weather and Space Climate
Referee for the following commissions:
US Energy division

TEACHING AND SUPERVISION ACTIVITY

Teaching

06/2019-07/2019: Lecturer at Space Summer School, organized by the Belgian Nuclear Research Centre SCk-CEN (www.sckcen.be)
10/2012 : mini-course on *"An introduction to TDDFT and linear response",* VUB, Brussels
2008: Qualification "Maitre de conferences" Sect. 28, 30, 31, Conseil National des Universites, France
2006: training/preparation of the examination for access/correction for students willing to enter the Optics and Optometry degree course at Univ. Roma Tre, Rome
2003/2004/2005/2006 : training for students willing to enter the Physics degree course at Univ. Roma Tre, Rome
09/2004-12/2004: practical lessons to 2nd year students for the course 'Electromagnetism' , Univ. Roma Tre, Rome
09/2003-12/2003: practical lessons to first year students for the course 'Calculus 1' , Univ. Roma Tre

Supervision

2013: Supervision of the PhD student Niko Van den Brande (VUB, Brussels) about TDDFT studies on organic solar cells with range-separated functionals
2012-2013: Supervision of the PhD student Zino Boisdenghien (VUB, Brussels) for fundamental studies about the local polarizability of single atoms
2011: Assisting Prof. D. Lamoen of the University of Antwerp with some students of the bacherol level, for small projects on electronic structure calculations on TiO2
2006: during my PhD, I co-supervised the MSc. student Eleonora Aquilini, University Roma Tre, Thesis's title: ¨The correlated motion of Auger electrons in angular momentum theory¨.

ORGANIZATION OF CONFERENCES/WORKSHOPS/ EVENTS

Conferences, Workshops

Workshop "Modelling the biological effects of radiation: from Earth studies to Space and Planetary Exploration" , 28-29/03/2019, Lille, France
Workshop "Enabling Smart Computations to study Space Radiation Effects" , 1/06/2018, Brussels, Belgium
"International Conference on Many particle spectroscopy of atoms, molecules , clusters and surfaces" 22-24/06/2006, Rome, Italy

Outreach Events

Open Doors Royal Belgian Institute for Space Aeronomy, 29-30th September 2018, Brussels
Event" "Let's talk about Mars!, 9th May 2019, Planetarium, Brussels

INTERVIEWS ABOUT MY RESULTS / HIGHLIGHTS IN THE PRESS / COVERS OF JOURNALS

Interviews with Journalists and highlights in the press about my research results

- Scientific American
http://www.scientificamerican.com/article.cfm?id=vermillion-red-paint-darkening-physics
- Physics Focus
http://physics.aps.org/articles/v6/124
- Chemistry world
http://www.rsc.org/chemistryworld/2013/10/mercury-dark-influence-art-red-black-vermilion
- Physics Today
http://scitation.aip.org/content/aip/magazine/physicstoday/news/10.1063/pt.5.7023
- Chemical and Engineering News (C&EN)
http://cen.acs.org/articles/91/i47/Vermilions-RedGray-Transformation.html?h=-2122674036

Cover stories of journals

2015: Cover-Story for the EUSPEC newsletter: "Unexpected spin-orbital entanglement in Iron"
2013: Cover of journal: Casting light on the darkening of paintings, F. Da Pieve et al., PRL 111, 208302
2013: Cover of journal: Aberration-corrected microscopy for doped detonation nanodiamond , S. Turner, F. Da Pieve, et al., Phys. Stat. Sol. (a), 210, 1976 (2013)

PERSONAL SKILLS

Mother tongue(s) Italian

Other language(s)

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
English	C2	C2	C2	C2	C2
French	C2	C2	C2	C2	C1

Levels: A1/A2: Basic user - B1/B2: Independent user - C1/C2 Proficient user
Common European Framework of Reference for Languages

Communication skills

Excellent communication skills gained through my experience as:
- invited and normal speaker at conferences/workshops
- lecturer
- dissemination and outreach activities
- meetings at European Agencies in the context of H2020/FP7 projects, meetings with members of the Italian Government and Minister of Defense

Organisational / managerial skills

- Leadership : currently responsible of a team of 3 people at my Institute + supervision of the three postdocs hired at the sites of the partners of the consortium of the H2020 project I am leading (Queen's University of Belfast, UK, and nanoGUNE research centre in San Sebastian ES)
- Organisational: frequent organization of workshops and meetings, for both research networks and formal occasions with government members, members of the Research Executive Agency of the European Commission; assistance of the invited speakers at workshops/meeting at all levels (transport, hotel reservations); responsible for the organization of series of seminars during my PhD.

Job-related skills

Strong learning agility, abstract thinking, responsibility for relationships and capability to work in teams and independently as well. I am used to work in an international environment (both European and non-European). I generally try to develop myself as I develop my career, learning my strengths and weaknesses, and I always try to mix efficiency with personal creativity.

Digital skills

SELF-ASSESSMENT				
Information processing	Communication	Content creation	Safety	Problem solving
Independent User	Independent User	Independent User	Independent User	Independent User

- Coding: C, C++, Fortran, Python
- OS: Linux, Windows
- Experience with High Performance Computing (HPC) use and testing of highly parallelized codes
- Use of AI (Machine-learning tools) to find patterns (beginner)
- Excellent command of office suite (word processor, spread sheet, presentation software)
- Excellent command of photo editing software gained as an amateur photographer

Other skills

- Photography, Volleyball

Driving licence Category: B

PUBLICATIONS

articles in preparation

Radiation environment and doses for human explorers in future astrobiology-driven missions on Mars
F. Da Pieve, E. Botek, V. Pierrard, A.C. Vandaele, G. Gronoff+ESC2RAD team
Radiation Shielding of biological targets by new composite materials: relevance for Low Earth Orbit and interplanetary missions
E. Botek, V. Pierrard, A.C. Vandaele, ….. and F. Da Pieve
Complexity of amino acids from meteoritic findings: an information-theory approach to phase-change reactions
F. Da Pieve

publications in peer reviewed journals:

28. Recent developments of the ABINIT software package
X. Gonze, F. Jollet, F. Abreu Araujo, D. Adams, B. Amadon, T. Applencourt, … F. Da Pieve et al., Computer Physics Communications 205, 106 (2016) Impact Factor: 3.635
27. Fingerprints of entangled spin and orbital physics in itinerant ferromagnets via angle resolved resonant photoemission
F. Da Pieve
Phys. Rev. B 93, 035106 (2016) Impact Factor 3.718
26. Gap State imaging and spin-orbit effects in resonant photoemission
P. Krüger and F. Da Pieve,
Surface and Interface Analysis 48, 1169 (2016)
25. Colour degradation of artworks: an ab-initio approach of X-ray, electronic and optical spectroscopy analyses of vermilion photodarkening
C. Hogan and F. Da Pieve
J. Analitical Atomic Spectrometry 30, 588 (2015) Impact Factor 3.379
24. The Local Polarizability of Atoms and Molecules: a Comparison Between a Conceptual Density Functional Theory Approach and Time Dependent Density Functional Theory
Z. Boisdenghien, S.Fijas, F. Da Pieve, F. De Proft and P. Geerlings
Mol. Phys. 113, 1890 (2015) Impact Factor 1.837
23. Interstellar condensed (icy) amino acids and precursors: theoretical absorption and rotational spectra under UV and soft X-ray irradiation
F. Da Pieve, G. Avendano-Franco, F. De Proft and P. Geerlings
Monthly Notices of the Royal Astronomical Society 440 (1): 494 (2014) Impact Factor: 5.521
22. A Time Dependent DFT Study of the Efficiency of Polymers for Organic Photovoltaics at the Interface with PCBM
N. Van den Brande, G. Van Lier, F. Da Pieve, G. Van Assche, B. Van Mele, F. De Proft, P. Geerlings,
RSC Advances 4, 52658 (2014) Impact Factor: 3.289
21. Electronic structure calculations of mercury mobilization from mineral phases and photocatalytic removal from water and the atmosphere
F. Da Pieve, M.Stankovski and C. Hogan
The Science of Total Environment 493, 596 (2014) Impact Factor: 3.789
20. Casting light on the darkening of historical paintings
F. Da Pieve, C. Hogan, M. Radepont, F. Vanmeert, M. Cotte, J.Verbeeck, K. Janssens, D. Lamoen X. Gonze and G.Van Tendeloo
Phys. Rev. Lett. 111, 208302 (2013) Impact Factor: 7.645
19. First-principles calculations of Angle-Resolved and Spin-resolved photoemission Spectra of Cr(110) surfaces at the 2p-3d Cr resonance,
F. Da Pieve and P. Krüger
Phys. Rev. Lett. 110, 127401 (2013) Impact Factor: 7.645
18. Real space Green's function approach to angle-resolved resonant photoemission: spin polarization and circular dichroism in itinerant magnets
F. Da Pieve and P. Krüger
Phys. Rev. B 88, 115121 (2013) Impact Factor: 3.718
17. Origin of magnetism and quasiparticles properties in Cr-doped TiO2
F. Da Pieve, S. Di Matteo, T. Rangel, M. Giantomassi, D. Lamoen, G.-M. Rignanese and X. Gonze,
Phys. Rev. Lett. 110, 136402 (2013) Impact Factor: 7.645

16. Aberration-corrected microscopy and spectroscopy analysis of N-doped detonation nanodiamond
S. Turner, O. Shenderova, F. Da Pieve, E. Yücelen, D. Lamoen, J. Verbeeck and G. Van Tendeloo
Phys. Stat. Sol. (a), 210, 1976 (2013) Impact Factor 1.21

15. Spin-dependent on-site electron correlations and localization in itinerant ferromagnets
R. Gotter, G. Fratesi, R. A. Bartynski, F. Da Pieve, F. Offi, A. Ruocco, M. I. Trioni, G. P. Brivio, G. Stefani
Phys. Rev. Lett. 109, 126401 (2012) Impact Factor: 7.645

14. Analysis of the Local Boron Environment in Boron-doped Nanocrystalline Diamond Films,
S.Turner, Y. Lu, S. D. Janssens, F. Da Pieve, D. Lamoen, J. Verbeeck, K. Haenen, P. Wagner and G. Van Tendeloo
Nanoscale 4, 5960 (2012) Impact Factor: 6.233

13. MsSpec-1.0 : a multiple scattering package for electron spectroscopies in material science
D. Sébilleau, C. Natoli, M. Gavaza, H. Zhao, F. Da Pieve, K. Hatada,
Comput. Phys. Commun. 182, 2567 (2011) Impact Factor: 3.635

12. Evidence for the collapse of shart-range magnetic order in CoO at the Neel temperature,
R.Gotter, F.Offi, A. Ruocco, F. Da Pieve, R.Bartynsky, M.Cini and G.Stefani,
European Physics Letters 94, 37008 (2011) Impact Factor: 2.753

11. Real-space multiple scattering method for angle-resolved photoemission and valence band photoelectron diffraction and its application to Cu(111),
P.Krüger, F. Da Pieve and J.Osterwalder
Phys. Rev. B 83, 115437 (2011) Impact Factor: 3.718

10. M3M45M45 Auger lineshape measured from the Cu(111) surface: Multiplet term selectivity in angle-resolved Auger-photoelectron coincidence spectroscopy,
R. Gotter, F. Da Pieve, F. Offi, A. Ruocco, A. Verdini, H. Yao, R. Bartynski, and G. Stefani,
Phys. Rev. B 79, 075108 (2009) Impact Factor: 3.718

9. Multiple scattering approach to two-electron resonant emission from solids,
F. Da Pieve, S. Di Matteo, D. Sebilleau, R. Gunnella, G. Stefani and C.R. Natoli
Phys. Rev. B 78, 035122 (2008) Impact Factor: 3.718

8. Angular correlation between photoelectrons and Auger electrons within scattering theory,
F. Da Pieve, S. Di Matteo, D. Sebilleau, R. Gunnella, C.R. Natoli and G. Stefani,
Phys. Rev. A 75, 052704 (2007) Impact Factor: 2.861

7. Linear Magnetic and Alignment Dichroism in Auger-photoelectron Spectroscopy,
F. Da Pieve, S.Fritzsche, G.Stefani and N.M.Kabachnik,
J. Phys. B: At. Mol. Opt. Phys. 40, 329 (2007) Impact Factor: 1.902

6. Study of electronic correlations in the Auger cascade decay from Ne*1s-13p,
F. Da Pieve, L.Avaldi, R.Camilloni, M.Coreno, A.Ruocco, S.Fritzsche, N.Kabachnik, G.Stefani,
J.Phys. B: At., Mol., Opt. Phys. 38, 3619 (2005) Impact Factor: 1.902

5. Dichroic effects in Auger-photoelectron coincidence spectroscopy (APECS) from solids,
R.Gotter, F. Da Pieve, A.Ruocco, F.Offi, G.Stefani and R.Bartynski,
Phys. Rev. B 72, 235409 (2005) Impact Factor: 3.718

conference proceedings (peer-reviewed):

4. Spin selectivity by Auger Photoelectron coincidence spectroscopy,
S. Ugenti, M. Cini, E. Perfetto, F. Da Pieve, C.R. Natoli, R.Gotter, F.Offi, A.Ruocco, G.Stefani,
F. Tommasini, G.. Fratesi, M.I.Trioni and G.P.Brivio,
J. Phys.: Conf. Ser. 100 072020 (2008) This Proceeding journal is not issued with Impact Factor

3. Electronic and magnetic properties of thin films probed by Auger-photelectron coincidence spectroscopy (APECS) ,
R.Gotter , F.Offi, F. Da Pieve, A.Ruocco, G.Stefani, S.Ugenti, M.I.Trioni, R.Bartynsky,
Journal of Electron Spectroscopies and Related Phenomena 161 , 128 (2007) Impact Factor : 1.750

2. Photoelectron-Auger electron coincidence study for condensed matter
G.Stefani, R.Gotter, A.Ruocco, F.Offi, F. Da Pieve, S.Iacobucci, A.Morgante, …H.Yao and R.Bartynsky,
Journal of Electron Spectroscopies and Related Phenomena 141, 149 (2004) Impact Factor : 1.750

book chapter (peer-reviewed):

1. Relevance of the core hole alignment to Auger photoelectron pair angular distribution in solids,
in “Correlation Spectroscopies of Surfaces, Thin Films, and Nanostructures”,
G. Stefani, R. Gotter, A. Ruocco, F. Offi, F. Da Pieve, A. Verdini, A. Liscio, S. Iacobucci, H. Yao,
R. Bartynski, edited by J.Kirschner and J. Berakdar (2004)

SEMINARS

Invited Seminars at Conferences/Workshops

Space Weather research and applications (2"rd April 2019, Brussels, Belgium)
"Radiation risks during future human exploration of Mars and challenges in the search of new shielding solutions"
Towards understanding and modelling intense electronic excitations, TUMIEE cost action workshop CA 17126 (19-20th November, Madrid, Spain)
"Space Radiation at candidate landing sites for the ExoMars 2020 ESA mission: a Monte Carlo study"
Formation of the Solar System and the Origin of Life (20-24th February 2017, Leiden, The Netherlands)
"Photophysics of condensed amino acids and precursors under UV radiation from state-of-the-art theoretical spectroscopy"
Electron Correlations: from Gases to Solids (ElCoGS 2017) (8-9th June 2017, Rome, Italy)
"Spectroscopy of organic matter from space: investigating the origin of preferred chirality in life"
EMN workshop, Energy Materials and Nanotechnology (1-4th September 2015, San Sebastian, Spain)
"Fingerprints of spin and orbital physics in metals via resonant photoemission"
Meeting of the Contact group for Synchrotron Radiation of F.R.S.-FNRS (8-9th December 2014, Namur, Belgium)
"Correlation effects in absorption, photoemission and light scattering spectroscopies: present status of theoretical approaches and new challenges"
Workshop EuSpec: Modern Tools for Spectroscopy on Advanced Materials (15-17th September 2014, Louvain La Neuve, Belgium)
*"Multiexcitonic effects and spin-orbital excitations in RIXS: an ab-initio ROAD MAP"*Recent advances in spectromicroscopy: experimental and theoretical tools
Recent advances in spectromicroscopy: experimental and theoretical tools (3-6/09 2013, Mons, BE)
"The impact of the highly improbable: homochirality and circular dichroism in astrophysical contexts"
Designing novel materials for nanodevices: From Theory to Practice (9th-12th December 2012, Helmholtz Zentrum Berlin - Bessy II, Berlin, Germany)
"*Native defects in photocatalysts: an insight from many body theory"*
Magnetic order in nanostructures and spectroscopy (MONAS) (13-15th September 2012, Rome, Italy)
"*Local magnetic properties probed by spin and angle resolved resonant photoemission via first-principles"*
Nano-TP Workshop (23 october 2012, Dubendorf, Switzerland)
¨*Theory and microscopy for environmental science: identification of the sources of environmental pollution and possible photocatalysts for decontamination*¨
14th International Conference on X-ray Absorption Fine Structure (XAFS14) (26-31th July 2009, Camerino, Italy)
"*Spin polarized dichroism in resonant photoemission on Fe"*
14th International Symposium on Polarization and Correlation in Electronic and Atomic Collisions (1-4th August 2007 Königstein, Germany)
"*Recent advances and new perspectives in Auger-photoelectron angular correlations in atoms and solids"*

Seminars as Normal Participant at Conferences/Wprkshops

European Geophysical Union Conference 2019 (8-12th April 2019, Wien)
"Radiation environment and Habitability on Mars at Oxia Planum and Mawrth Vallis: influence of mineralogy, atmospheric depth and Solar activity"
Astrobiology: from stars and planets to extreme life, FNRS meeting (18th December 2018, Liège)
"The search of habitable conditions on Mars from the perspective of the radiation environment: influence of mineralogy and atmospheric depth through epochs"
European Planetary Science Conference 2018 (17-21st September 2018, Berlin)
"Radiation environment at candidate landing sites on Mars: effects of Solar activity and diurnal variations for different mineralogical content"
European Planetary Science Conference 2018 (17-21st September 2018, Berlin)
"Towards new strategies for biosignatures detection: correlating the chemical-physics properties and the complexity of amino acids from deep space"
51st ESLAB Symposium: Extreme Habitable Worlds (4th-8th December, 2017, ESA-ESTEC)
"Response of potential new solar cells on the surface of Mars for assessing future habitability: a space weather and materials modelling study"

Information Universe Conference (7th-9th October, 2015, Groningen, the Netherlands)
"Understanding the information content and the homochirality of the building blocks of life via theoretical spectroscopy"
Meeting of the F.R.S.-F.N.R.S. Contact group for Synchrotron Radiation (12th-13th November, 2015, Namur, Belgium)
"Precursor instabilities and enhancement of local correlations in itinerant magnetic systems via angle resolved photoemission"
Life in a Cosmic Context (15th-17th September 2015, Trieste, Italy)
"Circular dichroism on condensed amino acids and precursors: results from Time Dependent Density Functional Theory"
CORPES15, International workshop on strong correlations and angle-resolved photoemission spectroscopy
(5th -10th July 2015, Paris, France)
"Probing the Atomic Scale Magnetic Structure via Spin-flip, Orbital-flip and Chiral Excitations in Resonant Photoemission"
CHARM workshop, Contemporary physical challenges for Heliospheric and AstRophysical Models (18th -19th September 2014, Brussels, Belgium)
"Turbulence-induced orbital momentum in starlight: a source for a new type of light-matter interaction"
International Conference on Advanced Material Modelling (ICAMM 2014) (7-9th July 2014, Nantes, France)
"On mirrors, shadows, and the origin of life"
Workshop on fundamental aspects of X-ray spectroscopies: the role of 2p core hole in XAS and RIXS (21-22nd february 2013, Utrecht, Holland)
"Spin polarized resonant ARPES at the L23 edges of antiferromagnets and paramagnets"
Recent progress in Dynamical Mean-Field Theory and GW calculations (17-20th December 2012, Strasbourg, France)
"Spin polarized resonant ARPES: local properties in antiferromagnets and paramagnets"
Meeting of the Belgian Physical Society (30th May 20102, Vrije Universiteit Brussel, Belgium)
"Casting light on the darkening of colours in historical paintings"
ETSF Young Researcher Meeting (21-25th May 2012, Brussels, Belgium)
"Visible light absorption and magnetism in doped TiO2: a many body perturbation theory and spin - orbital hamiltonian analysis"
76th Annual Meeting of the Deutsche Physikalische Gesellshaft e.V. and DPG Spring Meeting (25-30th March 2012, Berlin, Germany)
¨Origin of magnetism and quasiparticle properties of Cr-doped rutile and anatase TiO2¨
Challenges in Density Matrix and Density Functional Theory (1-6th April 2012, Ghent,Belgium)
¨DFT and Many body Perturbation Theory at work for art: understanding colours in historical paintings¨
17th WIEN2k workshop and International Conference on Advanced Material Modelling (ICAMM 2010) (5-10th July, 2010, Nantes, France)
¨Electronic, magnetic and optical properties of TiO2 with selective doping: DFT and beyond'
International Workshop on X-ray spectroscopy of Magnetic Solids (10-11th June 2010, Diamond Light Source, UK)*"Spin polarized dichroism and local magnetic moments from resonant photoemission: a band picture"*
ABINIT Workshop (24-27th March 2009, Autrans, France)
"Implementation of Raman scattering for spin polarized systems"
XIII SILS, Congress of the Italian Society for Synchrotron Radiation, (6-8th July 2006, Naples, Italy)
"Two electron resonant emission in the multiple scattering process"
ECASIA 2005, 11th European Conference on Applications of Surface and Interface Analysis (25-30th September 2005, Wien, Austria)
"Spin selectivity from solids with Auger- photoelectron coincidence spectroscopy"
MMD meeting, Matter and Material Devices meeting (22-25th June 2005, Genova, Italy)
"Auger-Photoelectron coincidence spectroscopy as a technique to probe the spin of atoms in solids"
XII SILS, Congress of the Italian Society for Synchrotron Radiation, (5-8th July 2004, Camerino, Italy)
"Photoelectron-Auger electron coincidence study of Sn/Ge(111): role of the magnetic sublevels"

Invited Seminars at Universities/Research Institutions

"Modelling the biological damage of human explorers on Mars and during deep Space travel"
7th February 2019, Queen's University of Belfast, UK
"*Chemical-physics properties, complexity and chirality measures for the amino acids of the isoleucine series from Antarctic meteorites"*
7th November 2018, University of Cambridge, Cavendish Laboratory
"Fingerprints of entangled spin and orbital physics in itinerant systems via resonant photoemission"
27th October 2015, European Synchrotron Radiation Facility (ESRF), Grenoble, France
"*Applications of theoretical spectroscopy: from condensed matter to astrophysical problems"*
12th February 2014, King's College, London
"*What theoretical spectroscopy is all about: from condensed matter to astrophysical problems",*
September 2013, ULB, Université Libre de Bruxelles, Belgium
"New routes for spintronics: room temperature ferromagnetism in dilute magnetic oxides"
12th October 2012, University of Mons
"New routes for spintronics: from dilute magnetic oxides to diffraction through chiral structures"
University of Namur, 18th September 2012
"Doping transition metal oxides: an ab-initio many body and spin orbital Hamiltonian perspective"
University Roma Tre, Physics Department, Rome, Italy, April 2012
¨Electronic properties studied by electron emission spectroscopies¨ University of Antwerp, Antwerp, Belgium, 29th January 2010
"Multiple scattering approach for the interpretation of spectroscopic results" Free University of Berlin, group of Prof. E.K.U. Gross, May 2008
¨Resonant Double Electron Emission Studied by Coincidence Spectroscopy¨ University of Rennes, Rennes, France, 3rd October 2005

europass Curriculum vitae

Stefano Iubini

ATTIVITÀ DI RICERCA

01/12/2017 - oggi
Assegnista di ricerca presso Università degli studi di Padova
tema della ricerca: Trasporto di materia e viscoelasticità in sistemi complessi
collaborazione con: Prof. Marco Baiesi (Università di Padova)
tipologia contratto: Assegno di ricerca - art 22 Legge 240/2010, N. 3077 16/11/2017

01/12/16 - 30/11/2017
Assegnista di ricerca presso Università degli studi di Firenze
tema della ricerca: studi teorici delle proprietà di trasporto di calore di sistemi con interazione a lungo raggio
collaborazione con: Prof. L. Casetti e Prof. R. Livi (Università di Firenze)
tipologia contratto: Assegno di ricerca - art 22 Legge 240/2010, N. 169186(1724) 29/11/2016

01/02/2014 - 30/11/2016
Postdoc presso Centre de Biophysique Moleculaire - CNRS Orleans (Francia)
tema della ricerca: Studi teorici e numerici delle proprietà di trasporto energetico in proteine
collaborazione con: Prof F. Piazza (CNRS Orleans)
tipologia contratto: dal 01/02/14 al 31/01/16 contratto di postdoc, N. 451768 31/01/2014 - dal 01/02/16 al 30/11/16 contratto di ricercatore a tempo determinato, N. 576511 22/01/2016 e N. 609876 17/08/2016

01/01/2011 - 31/12/2013
Dottorato di ricerca, Università di Firenze (XXVI ciclo)
tema della ricerca: Studi teorici e numerici di proprietà di trasporto in reticoli nonlineari
tutor: Dr. Stefano Lepri (Istituto dei Sistemi Complessi - CNR Firenze)
tipologia contratto: borsa di dottorato

01/07/2010 - 31/12/2010
Assegno di ricerca - Istituto dei Sistemi Complessi, CNR Firenze
tema della ricerca: Studi teorici e numerici di problemi termodiffusivi
collaborazione con: Prof. A. Politi (Istituto dei Sistemi Complessi, CNR Firenze)
tipologia contratto: Assegno di ricerca - Art 51 comma 6 legge 449/97, N. 0001424 28/06/2010

TITOLI DI STUDIO

Dottorato di ricerca in Fisica e Astronomia, Università degli studi di Firenze
Titolo della tesi: The nonequilibrium discrete nonlinear Schrödinger equation
Tutor: Dr. S. Lepri (Istituto dei Sistemi Complessi - CNR, Firenze)
Titolo conseguito in data: 20/01/2014

Laurea Specialistica in Scienze Fisiche e Astrofisiche, Università degli studi di Firenze
Indirizzo: Fisica Teorica
Tipologia: 20/S - classe delle lauree specialistiche in fisica (D.M. 28/11/2000)
Titolo della tesi: Proprietà dinamiche e termodinamiche dell'equazione di Schrödinger nonlineare discreta
Relatore: Prof. R. Livi (Università di Firenze, Dipartimento di Fisica e Astronomia)
voto: 110/110 con lode

Titolo conseguito in data	27/04/2010

Laurea Triennale in Fisica, Università degli studi di Firenze

Indirizzo	Scienze Fisiche
Tipologia	25 - classe delle lauree in scienze e tecnologie fisiche (D.M. 4/8/2000)
Titolo della tesi	Solitoni topologici in teorie classiche di campo
Relatore	Prof. R. Giachetti (Università di Firenze, Dipartimento di Fisica e Astronomia)
voto	110/110 con lode
Titolo conseguito in data	11/12/2007

Maturità scientifica, Liceo Scientifico “Amedeo di Savoia Duca d’Aosta” Pistoia (PT)

voto	100/100
Titolo conseguito nell’anno	2004

ABILITAZIONI

Abilitazione universitaria Francese

Tipologia specifica	Qualification à Maître de conférences
Sezione	28 “Milieux denses et matériaux”
Numero	15228276122
Data	05/02/2015

Abilitazione universitaria Francese

Tipologia specifica	Qualification à Maître de conférences
Sezione	29 “Constituants élémentaires”
Numero	18229276122
Data	02/02/2018

TEMI DI RICERCA

Parole chiave • Meccanica statistica di nonequilibrio • Dinamica non lineare • Sistemi complessi • Biofisica teorica • Sistemi magnetici

PUBBLICAZIONI IN RIVISTE PEER-REVIEWED

Nota: Il numero di citazioni (N.C.) riportato in fondo ad ogni elemento della lista è stato ottenuto da Google Scholar. L' *h* index risultante è 8. Per ogni elemento è altresì riportato l'impact factor (I.F.) della rivista (anno 2017).

17. **S. Iubini**, L. Chirondojan, G.-L. Oppo, A. Politi, P. Politi, *Dynamical freezing of relaxation to equilibrium*, *Physical Review Letters*, **122**, 084102 (2019) N.C. 2, I.F. 8.839
16. **S. Iubini**, E. Orlandini, D. Michieletto, M. Baiesi, *Topological sieving of rings according to their rigidity*, *ACS Macro Letters*, **7**, 1408-1412 (2018) N.C. 1, I.F 6.131
15. P. Di Cintio, **S. Iubini**, S. Lepri, R. Livi, *Transport in perturbed classical integrable systems: the pinned Toda chain*, *Chaos Solitons and Fractals*, **117** 249-254 (2018) N.C. 2, I.F. 2.213
14. **S. Iubini**, P. Di Cintio, S. Lepri, R. Livi, L. Casetti, Heat transport in oscillator chains with long-range interactions coupled to thermal reservoirs, *Physical Review E* (Editors' suggestion), **97** 032102 (2018) N.C. 3, I.F. 2.284
13. S. Pouyandeh, **S. Iubini**, S. Jurinovich, Y. Omar, B. Mennucci, F. Piazza, *Exciton transport in the PE545 complex: insight from atomistic QM/MM-based quantum master equations and elastic network models*, *Physical Biology*, **14** 066001 (2017) N.C. 2 I.F. 1.621
12. **S. Iubini**, S. Lepri, R. Livi, G.-L. Oppo, A. Politi, *A Chain, a Bath, a Sink and a Wall*, *Entropy*, 19(9), 445, (2017) N.C. 2, I.F. 2.305
11. S. Borlenghi, **S. Iubini**, S. Lepri, J. Fransson *Entropy production for complex Langevin equations*, *Physical Review E*, **96** 012150 (2017) N.C. 2, I.F. 2.284
10. **S. Iubini**, A. Politi, P. Politi, *Relaxation and coarsening of weakly-interacting breathers in a simplified DNLS chain*, *Journal of Statistical Mechanics*, **7** 073201 (2017) N.C. 3, I.F. 2.404
9. **S. Iubini**, S. Lepri, R. Livi, A. Politi, *Coupled transport in rotor models*, *New Journal of Physics*, **18** 083023 (2016) N.C. 4, I.F. 3.579
8. **S. Iubini**, O. Boada, Y. Omar, F. Piazza, *Transport of quantum excitations coupled to spatially extended nonlinear many-body system*, *New Journal of Physics*, **17** 113030 (2015) N.C. 14, I.F. 3.579
7. S. Borlenghi, **S. Iubini**, S. Lepri, J. Chico, L. Bergqvist, A. Delin, J. Fransson, *Energy and magnetisation transport in non-equilibrium macrospin systems*, *Physical Review E*, **92** 012116 (2015) N.C. 16, I.F. 2.284
6. S. Borlenghi, **S. Iubini**, S. Lepri, L. Bergqvist, A. Delin, J. Frannson, *Coherent energy transport in classical nonlinear oscillators: An analogy with the Josephson effect*, *Physical Review E - Rapid Communications*, **91** 040102(R) (2015) N.C. 10, I.F. 2.284
5. **S. Iubini**, S. Lepri, R. Livi, A. Politi, *Boundary-induced instabilities in coupled oscillators*, *Physical Review Letters*, **112** 134101 (2014) N.C. 8, I.F. 8.839
4. **S. Iubini**, A. Politi, P. Politi, *Coarsening dynamics in a simplified DNLS model*, *Journal of Statistical Physics*, DOI: 10.1007/s10955-013-0896-4 (2013) N.C. 10, I.F. 1.496
3. **S. Iubini**, S. Lepri, R. Livi, A. Politi, *Off-equilibrium Langevin dynamics of the discrete nonlinear Schrödinger chain*, *Journal of Statistical Mechanics*, P08017 (2013) N.C. 23, I.F. 2.404
2. **S. Iubini**, R. Franzosi, R. Livi, G.-L. Oppo, and A. Politi, *Discrete breathers and negative temperature states*, *New Journal of Physics*, **15** 023032 (2013) N.C. 24, I.F. 3.579
1. **S. Iubini**, S. Lepri, A. Politi, *Nonequilibrium discrete nonlinear Schrödinger equation*, *Physical Review E*, **86** 011108 (2012) N.C. 32, I.F. 2.284

PREPRINTS

- P. Di Cintio, S. Iubini, S. Lepri, R. Livi, *Equilibrium time-correlation functions of the long-range interacting Fermi-Pasta-Ulam model*, *ArXiv* 1901.04601 (2018)
- G. Teza, S. Iubini, M. Baiesi, A. L. Stella, C. Vanderzande, *Rate dependence of current and fluctuations in jump models with negative differential mobility*, *ArXiv*1904.05241 (2019)

SEMINARI E CONTRIBUTI A CONFERENZE

- 12-23 Novembre 2018, Ergodicity breaking in many body systems, International Institute of Physics, Natal Brazil - *1)"Tutorial on negative absolute temperatures"*, *2)"Frozen dynamics in the Discrete Nonlinear Schrödinger equation"* (Invited talks)
- 14-18 Ottobre 2018: Venice meeting on Fluctuations in small complex systems IV, Venice, *"Topological sieving of rings according to their rigidity"* (Poster)
- 13-14 Settembre 2018: Italian Soft Days 2018, Padova, *"Boundary-induced instabilities in coupled oscillators"* (Poster)
- 10-13 Settembre 2018: Non-equilibrium behaviour of classical and quantum systems, SISSA Trieste, *"Frozen dynamics in the Discrete Nonlinear Schrödinger equation "* (Talk)
- Luglio 2018: New trends in nonequilibrium statistical mechanics: classical and quantum systems - international school of statistical physics, Erice *Coupled transport phenomena in chains of oscillators"* (Invited Talk)
- Giugno 2018: International Conference on Nonlinear Localization in Lattices, Spetses (Greece) *"A chain, a bath, a sink and a wall"* (Talk)
- Maggio 2018: Advanced workshop on nonequilibrium systems in physics, geosciences and life sciences, ICTP Trieste *"Transport of topological probes in complex environments"* (Talk)
- 12-14 Aprile 2018: Convegno FPU2018, Scuola Galileiana Padova, *"Heat transport in FPU chains with long-range interactions"* (Invited Talk)
- Ottobre 2017: FisMat 2017, ICTP Trieste *"A chain, a bath, a sink and a wall"* (Talk)
- Settembre 2017: Thermodynamics and Statistical Mechanics of Small Systems, Roma Sapienza *"A chain, a bath, a sink and a wall"* (Poster)
- Giugno 2017: XXII Italian Conference on Statistical Physics, Università di Parma, *"A chain, a bath, a sink and a wall"* (Talk)
- Settembre 2016: International conference DICE 2016 spacetime - matter - quantum mechanics, Castiglioncello *Transport of quantum excitations coupled to spatially extended nonlinear many-body systems* (Talk)
- Giugno 2016: Enlight Workshop, Università di Pisa *Structural and dynamical determinants of exciton transport in coarse-grained models of light-harvesting complexes* (Talk)
- Giugno 2016: International workshop on Quantum Effects in Biological Systems, Durban, South Africa *Structural and dynamical determinants of exciton transport in coarse-grained models of light-harvesting complexes* (Talk)
- Settembre 2015: Biophys '15 From physics to biology and beyond, Università di Firenze, Firenze *"Energy transport in photosynthetic complexes: insights from coarse-grained semiclassical models"* (Invited Talk)
- Luglio 2015: International workshop on Quantum Effects in Biological Systems, Università di Firenze, Firenze *"The role of vibrations in exciton transfer: insights from coarse-grained semiclassical models"* (Talk + Poster)
- Giugno 2015: Molecular Quantum Dynamics Methods: Benchmarks and State of the Art, CECAM-HQ EPFL Lausanne, *"Exciton transfer and quantum efficiency in a 1D tight-binding model with local and non-local coupling to an explicit environment"* (Poster)
- Febbraio 2015: Good vibrations for Energy Management in Biomolecules, Lorentz Center, Leiden *"Quantum transport in a 1D tight-binding model with local and non-local coupling to an explicit environment"* (Poster)
- Ottobre 2014: Workshop on Non-Equilibrium Processes at Negative Temperature, University of Strathclyde, Glasgow, *"Stationary nonequilibrium processes at negative temperature"* (Talk)
- Settembre 2014: Instituto de Telecomunicações, Lisbon, *Discrete breathers and negative temperature states* (Talk)
- Giugno 2014: XIX Italian Conference on Statistical Physics, Università di Parma, *"A boundary-induced transition in chains of coupled oscillators"* (Poster)
- Ottobre 2013: From Dynamics to Statistical Physics and Back - Focus Workshop, MPIPKS Dresden, *"The nonequilibrium discrete nonlinear Schrödinger equation, stationary transport in the presence of dynamical barriers"* (Poster)
- Giugno 2013: XVIII Italian Conference on Statistical Physics, Università di Parma, *"Discrete breathers and negative temperature states"* (Invited Talk)
- Ottobre 2012: Advanced Workshop on Energy Transport in Low-Dimensional Systems: Achievements and Mysteries, ICTP Trieste, *"The Nonequilibrium Discrete Nonlinear Schrödinger Equation"* (Poster)
- Giugno 2012: XVII Italian Conference on Statistical Physics, Università di Parma, *"The Nonequilibrium Discrete Nonlinear Schrödinger Equation"* (Poster)
- Settembre 2010: Complexity in periodically structured systems - International workshop, MPIPKS Dresden, *"Dynamics and thermodynamics in the Discrete Nonlinear Schrödinger Equation"* (Poster)

- Giugno 2010: XV Italian Conference on Statistical Physics, Università di Parma, *"Dynamical and thermodymical properties of the Discrete Nonlinear Schrödinger Equation"* (Poster)

ALTRI SEMINARI

- Marzo 2018: Ciclo di seminari del dipartimento di Fisica dell'Università di Padova, *Discrete breathers and negative-temperature states*
- Maggio 2017: Ciclo di seminari "Seminari sulla Complessità", CNR Sesto Fiorentino (FI), *Coupled transport phenomena in chains of oscillators*
- Febbraio 2016: Meeting of the European project PAPETS, UCL London, *Normal-mode assisted exciton transport*
- Aprile 2016 Seminario teorico Instituto Superior Técnico, Lisbona *Breathers and metastable states in the Discrete Nonlinear Schroedinger Equation*
- Aprile 2016: Seminario teorico INFN Pisa *Stochastic and dynamic aspects of energy localization in nonlinear lattices with constraints*
- Luglio 2015: Meeting of the European project PAPETS, Università di Firenze, Firenze *"The role of vibrations in exciton transfer: insights from coarse-grained semiclassical models"*
- Marzo 2014: Meeting of the European project PAPETS, UCL London, *A semiclassical model for energy transfer in photosynthetic complexes*
- Marzo 2013: Ciclo of seminari "Seminari sulla Complessità", Università di Firenze, *Discrete breathers and negative temperature states*
- Maggio 2012: PhD Day, Università di Firenze, *The Nonequilibrium discrete nonlinear Schroedinger equation*
- Giugno 2011: Liceo scientifico Amedeo di Savoia duca d'Aosta, Pistoia, *Introduzione alla termodinamica a temperature negative*

VISITE A CENTRI DI RICERCA SU INVITO

- 3-13 Aprile 2019: Center for Theoretical Physics of Complex Systems (PCS) - Institute for Basic Science (IBS), Daejeon, Corea del Sud. Referente: Prof. Sergej Flach.
  Seminari e lezioni:
  1) "Thermodynamics of negative-temperature states" (lecture)
  2) "Localization and slow-relaxation phenomena in the Discrete Nonlinear Schroedinger Equation" (lecture)
  3) "Transport properties of the Discrete Nonlinear Schroedinger Equation" (seminario)

SCUOLE

Maggio 2018	"Summer school on nonequilibrium" - Leuven, Belgio
Maggio 2014	*Training week* del workshop "Advances in Nonequilibrium Statistical Mechanics: large deviations and long-range correlations, extreme value statistics, anomalous transport and long-range interactions" - Firenze
Luglio 2011	Summer school "Nonequilibrium statistical mechanics" - Montréal, Canada

ATTIVITÀ DIDATTICA

Ottobre 2018 - oggi	Attività di didattica integrativa per il corso di *Fisica biologica con complementi di matematica*, Università di Padova, Corso di Laurea in Biologia Molecolare (16 ore)
Ottobre 2017 - Settembre 2018	Docente-tutor del corso di *Fisica I*, Polo Universitario Aretino (Arezzo), (48 ore) in collaborazione con Politecnico di Milano
Marzo 2017 - Aprile 2018	Titolare del corso di *Matematica II*, Università di Firenze, Facoltà di Scienze Matematiche Fisiche e Naturali, Corso di Laurea in ottica e optometria (48 ore)
Gennaio 2016 - Giugno 2016	Titolare del corso di *Algèbre Linéaire*, Université d'Orléans (France), faculté de Droit Economie Gestion (40 ore)
2015 - 2016	Co-supervisione della tesi di dottorato di Sima Pouyandeh (dottorato in cotutela Università di Lisbona e Università di Orléans) assieme ai Prof. Francesco Piazza e Yasser Omar
2014 - 2016	Co-supervisione della tesi di dottorato di Simon Aubailly (Università di Orléans e CBM-CNRS Orléans) assieme al Prof. Francesco Piazza

CONOSCENZE INFORMATICHE

Solida esperienza nella simulazione numerica della dinamica dei sistemi complessi

Sistemi operativi	Linux, Windows
Linguaggi di programmazione	C, Fortran, Bash, Lammps
Programmi di calcolo numerico	Maple, Mathematica

CONOSCENZE LINGUISTICHE

Italiano	madre lingua
Inglese	ottima conoscenza scritta e orale
Francese	buona conoscenza scritta e orale

COLLABORAZIONI SCIENTIFICHE IN CORSO

Prof. Marco Baiesi, Dipartimento di Fisica e Astronomia, Università di Padova
Prof. Enzo Orlandini, Dipartimento di Fisica e Astronomia, Università di Padova
Prof. Attilio Stella, Dipartimento di Fisica e Astronomia, Università di Padova
Prof. Carlo Vanderzande, Dipartimento di Fisica, Università di Hasselt, Belgio
Prof. Roberto Livi, Dipartimento di Fisica e Astronomia, Università di Firenze
Prof. Anna Delin, KTH Royal Institute of Technology, Svezia
Dr. Stefano Lepri, Istituto dei Sistemi Complessi - CNR Firenze
Dr. Paolo Politi, Istituto dei Sistemi Complessi - CNR Firenze
Prof. Antonio Politi, Istituto di Matematica Pura e Applicata, Università di Aberdeen, UK
Prof. Gian-Luca Oppo, Dipartimento di Fisica, Università di Strathclyde, UK
Prof. Francesco Piazza, CNRS e Università d'Orléans, Francia
Prof. Satya Majumdar, LPTMS Paris Sud, Francia

ALTRE ATTIVITÀ

Reviewer per le riviste	*Physical Review Letters*, *Physical Review E*, *Physical Review A*, *Communications in Nonlinear Science and Numerical Simulation*

RICONOSCIMENTI INTERNAZIONALI

2017	Marie Sklodowska-Curie Actions Seal of Excellence for individual fellowships, European Union/European Commission. Project proposal 795144 "TACT" Theory and Applications of Coupled Transport phenomena

TEMI DI RICERCA

Processi termodiffusivi in reti di oscillatori non lineari

L'obiettivo principale di questa indagine è la caratterizzazione dei processi di trasporto accoppiato in modelli di oscillatori interagenti. Un esempio molto importante è rappresentato dall'equazione di Schrödinger Nonlineare Discreta (DNLS), dove la presenza di due quantità consevate (energia e norma) richiede uno studio approfondito dell'interazione tra le corrispondenti correnti conservate. L'equazione DNLS è un modello efficace per la descrizione del trasporto di particelle bosoniche quali fotoni in guide d'onda accoppiate, atomi freddi in trappole ottiche periodiche o magnoni in mezzi magnetici nonlineari. Un'altra classe di modelli che rientra in questo tipo di studi è rappresentata dai modelli di rotatori accoppiati (come il cosiddetto modello XY).

Grazie a metodi teorici e numerici appositamente sviluppati per questo tipo di fenomenologia, è stato possibile caratterizzare i processi di trasporto accoppiato attraverso una matrice di Onsager. Più precisamente, la dipendenza di tale matrice dai parametri termodinamici del modello (temperatura e potenziale chimico) ha permesso di identificare i regimi di trasporto più rilevanti. In particolare sono stati individuati dei nuovi regimi di trasporto anomalo prodotti da peculiari effetti dinamici su scala microscopica.

Discrete breathers in regimi fuori dall'equilibrio e stati termodinamici a temperatura negativa

Le soluzioni di tipo *discrete breather* sono eccitazioni nonlineari spazialmente localizzate tipiche della dinamica di numerosi modelli nonlineari discreti e con notevole rilevanza sperimentale. Alcuni di questi modelli (come l'equazione DNLS) ammettono un regime dinamico in cui gli stati *breather* sono spontaneamente creati indipendentemente dalla scelta della condizione iniziale. In tale regime, si pone il problema di come caratterizzare il comportamento termodinamico del sistema. A questo scopo sono stati sviluppati strumenti specifici per l'analisi della dinamica del sistema per tempi lunghi e, in particolare, per il problema del rilassamento all'equilibrio. È stato quindi possibile identificare un processo di congelamento dello stato di nonequilibrio prodotto dalla presenza di *breathers* di grande ampiezza. L'entità del rallentamento è tale da rendere la convergenza all'equilibrio del tutto inaccessibile persino su scale di tempo molto lunghe rispetto ai tempi propri del sistema. Complessivamente questo fenomeno costituisce un peculiare esempio di rottura di ergodicità indotto da fenomeni puramente dinamici. A seconda dei parametri dinamici del sistema, la fase metastabile può essere inoltre caratterizzata da una temperatura efficace negativa, rappresentativa di uno stato termodinamico dove l'entropia del sistema è una funzione localmente decrescente dell'energia totale.

Trasporto di eccitoni in complessi fotosintetici

La fotosintesi è un processo biologico fondamentale che fornisce la fonte primaria di energia per quasi tutte le forme di vita sulla Terra. Durante gli stadi iniziali di tale reazione, si assiste all'assorbimento di un fotone da parte di un pigmento situato all'interno del complesso fotosintetico. Ciò permette la creazione di uno stato molecolare eccitato (eccitone) che viene successivamente trasferito verso il *reaction center* del complesso, dove viene assorbito. L'energia estratta dall'eccitone viene quindi utilizzata per innescare un processo ultraveloce di separazione di carica essenziale per le reazioni chimiche successive. Degna di nota è la straordinaria efficienza quantica che caratterizza questi processi di conversione di energia sotto condizioni di illuminazione bassa: quasi 100%. A questo proposito, studi teorici e sperimentali hanno mostrato la rilevanza delle vibrazioni della matrice proteica per massimizzare l'efficienza di trasporto eccitonico. Al fine di studiare esplicitamente il ruolo della struttura proteica per la dinamica eccitonica, è stato sviluppato un approccio semiclassico fondato sull'integrazione numerica simultanea dell'equazione di Schrödinger per l'eccitone e le equazioni di Newton per la matrice proteica. Le due equazioni sono accoppiate attraverso un termine che mette l'eccitone in interazione con le vibrazioni della proteina (e viceversa). La complessità del sistema è stata inoltre ridotta descrivendo il complesso fotosintetico al livello di network coarse-grained di oscillatori nonlineari. Con questo approccio, la dinamica eccitonica è controllata da una Hamiltoniana *tight-binding* definita sui nodi della rete di oscillatori. Questa strategia permette di riprodurre in maniera fedele le principali caratteristiche dinamiche precedentemente ottenute da approcci tipo *master equation* per i gradi di libertà eccitonici. In più, permette di identificare i modi normali di vibrazione proteici che influiscono maggiormente sulla dinamica eccitonica. Infine, la presenza esplicita di termini di interazione nonlineari consente di esplorare una serie di effetti dinamici potenzialmente rilevanti per il problema, come il ruolo di eccitazioni di tipo *discrete breather*.

Trasporto di calore in sistemi con interazioni a lungo raggio	I sistemi macroscopici con interazioni a lungo raggio esibiscono proprietà termodinamiche inusuali, quali instabilità (e.g. collassi gravitazionali) o regioni a calore specifico negativo. Se negli ultimi anni è stato raggiunto un quadro sufficientemente chiaro del loro comportamento all'equilibrio, il problema della conduzione stazionaria di calore è rimasto quasi completamente inesplorato. In questo contesto, è stato effettuato uno studio teorico e numerico di setup genuinamente fuori equilibrio, concentrandosi su semplici modelli di oscillatori accoppiati. Tale approccio ha permesso di chiarire il ruolo del range delle interazioni microscopiche per la conducibilità termica macroscopica.
Viscoelasticità ed interazioni topologiche in mezzi complessi	I fluidi complessi, come le emulsioni o i gel, sono caratterizzati da una struttura molto ricca alla scala spaziale dei micron. Questa struttura può dar luogo a comportamenti viscoelastici, ovvero ad una risposta intermedia tra quella di un fluido viscoso e quella di un solido elastico. In questo ambito di ricerca, gli esperimenti standard di reologia (e.g. shearing macroscopico) non riescono a fornire informazioni precise sulle strutture microscopiche responsabili del comportamento complesso del sistema. Per comprendere più a fondo la relazione tra proprietà microscopiche e comportamento macroscopico del sistema, si è introdotto un metodo innovativo che permette di "risolvere" le proprietà viscoelastiche del mezzo attraverso lo studio del moto di sonde micrometriche con topologia non banale (nel caso più semplice anelli). Tali sonde possono diffondere liberamente nel mezzo oppure possono essere soggette a forze esterne come campi elettrici. Una giustificazione intuitiva di tale scelta è che le sonde possono rimanere stabilmente intrappolate nelle strutture irregolari del sistema a causa di vincoli di natura topologica. Studi preliminari recenti (in preparazione) hanno confermato numericamente l'efficacia delle sonde topologiche per lo studio delle proprietà microscopiche di sistemi di tipo gel.

CURRICULUM VITAE OF SAVIO LARICCHIA

Current position

From 14.09.2015

to present: Postdoctoral Research Associate at King's College London, London, U.K. under the supervision of Prof. Mark van Schilfgaarde and Dr. Nicola Bonini to work on the evaluation of forces, phonon dispersion curves, and the electron-phonon coupling at the Quasiparticle Self-consistent GW (QSGW) level of theory by means of an all-electron code in the FP-LMTO basis set formalism.

Education

31.03.2006: First level degree in Chemistry achieved at the Facolta' di SCIENZE MATEMATICHE FISICHE e NATURALI, Università degli studi di Bari with 110/110 *cum laude* with the thesis: **STOCHASTIC METHODS FOR THE SIMULATION OF THE NANOCRYSTAL GROWTH**.

02.04.2009: Master Degree in Chemical Science and Technology achieved at the Facolta' di SCIENZE MATEMATICHE FISICHE e NATURALI, Università degli studi di Bari with 110/110 *cum laude* with the thesis: **QUANTUM MECHANICAL SIMULATIONS OF THE SURFACE-MOLECULE INTERACTION**.

From 17.06.2010

to 17.06.2013: PhD in Theoretical and Computational Chemistry achieved at the Center for Biomolecular Nanotechnologies @UNILE, Italian Institute of Technology (IIT), Lecce, Italy.

Thesis title: **NEW DEVELOPMENTS IN SUBSYSTEM FORMULATION OF DENSITY FUNCTIONAL THEORY**

Supervisor: Dr. Ing. Fabio Della Sala

Research experience

From 1.06.2009

to 31.05.2010: winner of the scholarship at the National Nanotechnology Laboratory (NNL), Lecce, Italy. PROT. CNR-INFM 0007051 of the 19/05/2009, announcement BS 06/2009 of the 27/03/2009, Centro di Responsabilita' CNR-INFM, Unità Operativa di Lecce, CRS NNL, to carry out studies and research for the Grant Agreement with the U.E., Development of Density Functional Theory methods for Organic Metal Interaction (DEDOM) for the thematic *Simulation of organic molecules on metallic substrate*.

From 1.08.2013

to 31.09.2013: occasional collaboration contract at the CNR-NANOSCIENZE (Lecce, Italy) to carry out studies and research to extend the subsystem formulation of Density Functional Theory to fractional occupation numbers.

From 01.05.2014

to 15.06.2014: occasional collaboration contract at the CNR-NANOSCIENZE (Lecce, Italy) to carry out studies and research on an exact Subsystem DFT formalism in a constrained-orbitals non-orthogonal Kohn-Sham scheme.

From 16.06.2014

to 31.08.2015: Postdoctoral fellow at Temple University, Philadelphia (PA), U.S.A. under the supervision of the Profs. John Perdew (from 16.06.2014 to 31.12.2014) and Adrienn Ruzsinzky (from 16.06.2014 to 31.08.2015) to carry out studies on correlation energy from Adiabatic-Connection Fluctuation Dissipation (ACFD) theorem and development of self-correlation free non-local exchange-correlation kernels.

Teaching experience

18.09.2014: One-day teaching experience in Solid State Physic for the Ph.D. course in place of Prof. John Perdew at Temple University, Philadelphia (PA), U.S.A.

From 10.11.2015

to 11.01.2016: Assisting Prof. Francesca Baletto for the course 5CCP211C *Computational Laboratory* and marking for written and oral tests at the Physics Department of King's College London, London (U.K.)

Skills

Computer

Operating systems:

- Linux (good)

Quantum-chemistry softwares:

- QUESTAAL (good, developer; see https://www.questaal.org/)
- TURBOMOLE (good, developer)
- ABINIT (good,developer)
- QUANTUM ESPRESSO (good)
- GAMESS (fair)
- GAUSSIAN (fair)
- CFOUR (fair)

Programming languages and scripts:

- Fortran (good)
- C (good)
- Shell scripting (good)
- Python (beginner)

Languages

- Italian (mother tongue)
- English (fluent)

Research interests

scholarship (from 01/06/2009 to 31/05/2010) and Ph.D. (from 17/06/2010 to 17/06/2013)

My research interests was focused on the development of extensions of the Subsystem formulation of Density Functional Theory (DFT), an accurate (in principle exact) QM-QM embedding method. In particular my work was based on the following points:

- to find a better kinetic energy functional approximation required to compute the non-additive kinetic contribution to the embedding potential. My colleagues and I developed new PBE-like

kinetic energy functionals (APBEk and revAPBEk) using the *semiclassical neutral atom* as a reference system in DFT and rationalized their accuracy for Subsystem DFT applied to nonbonded interactions. We also developed laplacian-level kinetic energy functionals based on the fourth-order gradient expansion;

- to extend this approach to hybrid and orbital-dependent functionals in order to reduce the Self Interaction Error (SIE) and, therefore, the importance of the kinetic approximation (that depends on the extent of the density overlap between two or more interacting subsystems);
- to write a general Subsystem DFT formalism with non-integer subsystems' particle numbers, providing a deep insight into the role of the derivative discontinuity and of the chemical reactivity descriptors in such a context;
- to write an exact Subsystem DFT formalism in a constrained-orbitals non-orthogonal Kohn-Sham scheme (work still not published);
- I realized the first implementation of the subsystem DFT method in the TURBOMOLE program package which was realized in the script *FDE* (released in TURBOMOLE version 6.4).

Postdoctoral fellow at Temple University (from 16/06/2014 to 31/08/2015)

In this first postdoctoral experience my research interests focused on the evaluation of the correlation energy from Adiabatic-Connection Fluctuation Dissipation (ACFD) theorem and the development of a one-electron self-correlation free non-local exchange-correlation (xc) kernel exact for two electron systems in the high density limit. The implementation of the xc kernel correction to RPA and of the reciprocal-space wavevector symmetrization of any Homogeneous Electron Gas (HEG) exchange-correlation model kernel has been done in the ABINIT program package. The wavevector symmetrization of the xc kernel matrix in reciprocal space has been parallelized.

Postdoctoral Research Associate at King's College London (from 14/09/2015 to present)

In this second postdoctoral experience my research interest is focused on the evaluation of the phonon dispersion curves at the Quasiparticle Self-consistent GW (QSGW) level of theory by means of the QUESTAAL program package. QUESTAAL is a suite of all-electron codes for electronic structure simulations in the Full Potential Localized Muffin-Tin Orbital (FP-LMTO) basis set formalism. QSGW phonon frequencies are evaluated within the microscopic formalism for the Dynamical matrix where the static RPA inverse dielectric matrix is corrected by adding ladder diagrams through the solution of the Bethe-Salpeter equation. Then, the electron-phonon coupling (which can be a challenge in Density Functional Theory because of the implicit approximation of the inverse dielectric matrix) is evaluated in the Hedin-Lundqvist formalism at a many-body level

of theory. Furthermore, the mathematical formalism for the evaluation of the Dynamical matrix at the many-body level allows one to evaluate forces, so that the evaluation of the forces at the QSGW level of theory will be a consequent side effect of this project.

Publications

1) **S. Laricchia**, F. Ciriaco, L. Cassidei, F. Mavelli, DFT study of 1,3-Benzenedimethanethiol Adsorbtion on Au(111), *Sensor Lett.* **8**, 521-527 (2010)

2) F. Della Sala, E. Fabiano, **S. Laricchia**, S. D'Agostino, M. Piacenza, The role of exact-exchange in the theoretical description of organic-metal interfaces, *International Journal of Quantum Chemistry* **110**, 2162-2171 (2010).

3) **S. Laricchia**, E. Fabiano, F. Della Sala, Frozen density embedding with hybrid functionals, *J. Chem. Phys.* **133**, 164111 (2010).

4) Lucian A. Constantin, E. Fabiano, **S. Laricchia**, and F. Della Sala, Semiclassical Neutral Atom as a Reference System in Density Functional Theory, *Phys. Rev. Lett.* **106**, 186406 (2011).

5) **S. Laricchia**, E. Fabiano, Lucian A. Constantin, and F. Della Sala, Generalized Gradient Approximations of the Noninteracting Kinetic Energy from the Semiclassical Atom Theory: Rationalization of the Accuracy of the Frozen Density Embedding Theory for Nonbonded Interactions, *J. Chem. Theory Comput.* **7 (8),** 2439 (2011).

6) L. Chiodo, M. Salazar, A. Romero, **S. Laricchia**, F. Della Sala, and A. Rubio, TiO_2 atomic cluster, from structural to optical properties: an *ab initio* study, *J. Chem. Phys.* **135**, 244704 (2011).

7) **S. Laricchia**, E. Fabiano, and F. Della Sala, Frozen Density Embedding Calculations with the orbital-dependent localized Hartree-Fock Kohn-Sham potential, *Chem. Phy. Lett.* **518**, 114-118 (2011).

8) **S. Laricchia**, E. Fabiano, and F. Della Sala, On the accuracy of frozen density embedding calculations with hybrid and orbital-dependent functionals for non-bonded interaction energies, *J. Chem. Phys.* **137***,* 014102 (2012).

9) L. Chiodo, A. Massaro, **S. Laricchia**, F. Della Sala, R. Cingolani, M. Salazar, A. H. Romero and A. Rubio, Characterization of TiO_2 atomic crystals for nanocomposite materials oriented to optoelectronics, *Optical and Quantum Electronics.* **44**, 291 (2012).

10) **S. Laricchia**, E. Fabiano, and F. Della Sala, Semilocal and hybrid density embedding calculations of ground-state charge-transfer complexes, *J. Chem. Phys.* **138,** 124112 (2013).

11) A. Scrascia, L. De Marco, **S. Laricchia**, R. A. Picca, C. Carlucci, E. Fabiano, A. L. Capodilupo, F. Della Sala, G. Gigli, and G. Ciccarella, Fluorine-thiophene-substituted organic dyes for dye sensitized solar cells, *J. Mat. Chem. A* **1***,* 11909 (2013).

12) E. Fabiano, **S. Laricchia**, F. Della Sala, Frozen density embedding with non-integer subsystems' particle numbers, *J. Chem. Phys.* **140***,* 114101 (2014).

13) **S. Laricchia**, L. A. Constantin, E. Fabiano, F. Della Sala, Laplacian-level kinetic energy approximations based on the fourth-order gradient expansion: global assessment and application to the subsystem formulation of Density Functional Theory, *J. Chem. Theory Comput.* **10 (1),** 164 (2014).

14) S. Smiga, E. Fabiano, **S. Laricchia**, L. A. Constantin, F. Della Sala, Subsystem Density Functional Theory with meta-generalized gradient approximation exchange-correlation functionals, *J. Chem. Phys.* **142**, 154121 (2015).

15) Jefferson E. Bates, **S. Laricchia**, A. Ruzsinszky, Nonlocal energy-optimized kernel: Recovering second-order exchange in the homogeneous electron gas, *Phys. Rev. B* **93**, 045119 (2016).

16) K. Chen, B. Du, R. Zhang, C. Di Paola, **S. Laricchia**, N. Bonini, C. Weber, I. Abrahams, H. Yan, M. Reece, Enhanced thermoelectric performance of Sn-doped p-type Cu_3SbS_4, *J. Mater. Chem. C* **6**, 8546 (2018).

Invited talks

1) 19/11/2012 – 20/11/2012 Giulia Galli's group, University of California, Davis, California, USA.

2) 08/12/2014 Michele Pavanello's group, Rutgers University, Newark, New Jersey, USA.

3) 11/03/2019 seminar hosted by Stephan Lany, National Renewable Energy Laboratory, Golden, Colorado, USA.

Contributions to conferences

1) **S. Laricchia**, F. Ciriaco, L. Cassidei, F. Mavelli, DFT study of 1,3-benzenedimethanethiol adsorption on Au(111), presented at the *European Materials Research Society* (*E-MRS) 2009 Spring Meeting*, 8-12 June 2009, Strasbourg, France.

2) **S. Laricchia**, E. Fabiano, F. Della Sala, Subsystem formulation of DFT for hybrid and orbital-dependent exchange-correlation functionals, presented at the *14th International Density Functional Theory Conference Applications in Physics, Chemistry, Biology, Pharmacy*, 29 August – 2 September 2011, in Demokritos National Center for Scientific Research (NCSR), Athens, Greece.

3) Member of scientific board for the *13th European Theoretical Spectroscopy Facility (ETSF) Young Researchers' Meeting* at King's College London, 6-10 June 2016, London, UK. https://yrm2016.github.io/

4) Workshop on electron-phonon interaction, 22-24 May 2018, in Louvain-la-Neuve, Belgium.

5) **S. Laricchia**, N. Bonini, M. van Schilfgaarde, Electron-phonon coupling within Quasiparticle Self-consistent GW. *American Physical Society (APS) March meeting* , 04-08 March 2019, Boston, U.S.A..

Training schools

From 16.04.2008
to 16.04.2008: *Amsterdam Density Functional Workshop* held at the Computer Center of the CINECA, Casalecchio di Reno (Bologna), Italy.

From 08.09.2008
to 19.09.2008: *17*th *Summer school of parallel computing* held at the Computer Center of the CINECA, Casalecchio di Reno (Bologna), Italy.

From 07.05.2009
to 08.05.2009: *Techniques and tools for scientific programming on Linux/Unix* held at the Computer Center of the CINECA, Casalecchio di Reno (Bologna), Italy.

Personal information

Removed for anonymity reasons

Abilitazione Scientifica Nazionale (ASN) – Art. 16, c.1, Legge 240/10

02B1 Fisica Sperimentale della Materia – 2a Fascia (dal 10/04/2017 al 10/04/2023)
02B2 Fisica Teorica della Materia – 2a Fascia (dal 12/04/2017 al 12/04/2023)

Work experience

Dates	**1 Feb 2012 – Today**
Occupation or position held	**Senior Researcher, Quantum Information Group**
Main activities and responsibilities	Security analysis of real-world quantum key distribution (QKD) systems, theoretical and experimental aspects. Development of novel protocols for quantum communications. Analysis of experimental data. Contributor to the QKD standards set by the Industry Specification Group of the European Telecommunications Standards Institute (ETSI).
Name and address of employer	*Removed for anonymity reasons*
Type of business or sector	Research and Development, High-Tech, Semiconductors, Photonics
Dates	**1 Apr 2010 – 31 Mar 2012**
Occupation or position held	**Research Assignee with 5‰ grant No. 81001910439**
Main activities and responsibilities	Research on protocols for quantum communications; polarization/phase-drift control in optical fibers and "quantum hacking" of real components and devices.
Name and address of employer	Physics Division, School of Science and Technology, University of Camerino – Via Madonna delle Carceri 9, 62032 Camerino (MC), Italy
Type of business or sector	Higher Education, Scientific Research
Dates	**01 Apr 2009 – 31 Mar 2010**
Occupation or position held	**Research Affiliate – Postdoc**
Main activities and responsibilities	Research on "Secure communications with quantum mechanics". Collaboration with Prof. G. Casati (Insubria University) for the first international QKD transmission, between Como (Italy) and Chiasso (Switzerland). Our QKD system run on 8.75 km preinstalled Telecom fiber with a QKD protocol I developed in 2004.
Name and address of employer	Consorzio Nazionale Interuniversitario per le Scienze Fisiche della Materia - CNISM - via Ostiense 159, 00154 Roma, Italy
Type of business or sector	Scientific Research
Dates	**01 Feb 2006 – 31 Mar 2009**
Occupation or position held	**Research Affiliate – Postdoc**
Main activities and responsibilities	Theoretical development and experimental implementation of the QKD protocol I introduced in 2004. In February 2007 we demonstrated the first Italian fiber-based QKD outside the lab on a 400m optical fiber in the town of Camerino (MC), Italy.
Name and address of employer	Physics Division, School of Science and Technology, University of Camerino – Via Madonna delle Carceri 9, 62032 Camerino (MC), Italy
Type of business or sector	Higher Education, Scientific Research
Dates	**30 Oct 2005 – 31 Jan 2006**
Occupation or position held	**Senior Researcher**
Main activities and responsibilities	My office was to introduce Quantum Information and QKD to the company staff and help with the start-up of their quantum optics laboratory.
Name and address of employer	*Removed for anonymity reasons*

Type of business or sector	Applied Research & Development

Education & training

Dates	**18 Feb 2005**
Title of qualification awarded	**Dottorato di Ricerca in Fisica**
Principal subjects/occupational skills covered	Thesis: "Quantum Decoherence and Quantum Cryptography" (theoretical), with Prof. F. De Pasquale (Univ. of Rome "Sapienza") and Prof. S. Mancini (Univ. of Camerino).
Name and type of organisation providing education & training	University of Rome "Sapienza", P.zza Aldo Moro 5, Roma (Italy)
National/international level	Ottimo
Dates	**26 May 2000**
Title of qualification awarded	**Laurea in Fisica (vecchio ordinamento). Condensed Matter, Quantum Optics**
Principal subjects/occupational skills covered	Thesis: "Active Quantum Teleportation" (experimental), with Prof. F. De Martini and Prof. G. Di Giuseppe (Univ. of Rome "Sapienza").
Name and type of organisation providing education & training	University of Rome "Sapienza", P.zza Aldo Moro 5, Roma (Italy)
National/international level	110/110

Personal skills & competences

Mother tongue(s)	**Italian**
Other language(s)	**English**

Self-assessment

Understanding	Speaking	Writing
Independent user (B2)	Independent user (B2)	Proficient user (C1)

Scientific interests, competences & other	*Quantum*: Optics, Information, Cryptography, Security, Metrology, Repeaters, Decoherence; Fibers, Polarization and Phase Control; Solid State Physics. *Theoretical*: Deep knowledge of all quantum protocols, techniques and security proofs. Models for decoherence, optical noise, phase-drift. PMD compensation methods, passive bang-bang control and active feedback. Mean-field techniques for materials with ordered phase. Entanglement and Bell inequalities. Optomechanical systems. *Experimental*: Generation of entangled photons through spontaneous parametric down-conversion (SPDC) from most common lasers and nonlinear crystals. Single-photon and coincidence detection. Bell tests of non-locality. Most common single-photon detectors, I/O boards from NI, general acquisition electronics, LabVIEW, DLL design with C++. Numerical simulations with Matlab, Mathematica, Python.
Papers	More than **75 papers** (listed below) of which 2 on *Nature* and 3 on *Nature Photonics* in the last 6 years. Citations: **1448**, *h*-index: **20** (Scopus source).
Patents	**22 international patents** (20 published, 2 filed – listed below), of which 9 as first author.
Conferences	More than **20 talks** (16 invited, >4 contributed – partially listed below) in international conferences.

Projects	Author and Contributor to National, European and International projects: UK "Quantum Technology Hub for Quantum Communications Technologies" (2016, 24M£); European Project MIQC2 "Optical Metrology for Quantum-Enhanced Secure Telecommunication" (2015, 2M€); Japanese Project "Secure Photonic Network" (2012, 2.5M£); EU FP6 Integrated Project "QAP: Qubit Applications" (2006, 12M€); Italian Projects INNESCO: "Two-way quantum secure communication: from qubits to continuous variables" (2005); PRIN: "Generation, manipulation and detection of entangled light for quantum communication" (2004).
Reviewer	Reviewer for international journals like Nature, Nat. Photonics, Nat. Communications, Nat. Machine Intelligence, Light – Science and Applications, Scientific Reports (*NPG*); Phys. Rev. Lett. / X / A (*APS*); New Journal of Physics and Quantum Science & Technology (*IOP*); Optics Express, Optics Letters, JOSA B, Advances in Optics and Photonics (*OSA*); npj Quantum Information; Applied Physics Letters.
	Member of the Program Committee for QCrypt 2015 and QCrypt 2017.
Teaching experience	2006 – Today: co-supervisor of more than 15 PhD students.
May 2018	Lectures on "Measurement-Device-Independent Quantum Key Distribution" and "Industrial and Commercial aspects of Quantum Key Distribution", QCall Summer School, Baiona, Spain.
Apr 2016	Lecture for undergraduate students "An Introduction to Quantum Key Distribution", University of Vigo, Vigo, Spain
Jan 2012	Lectures for the course of "Meccanica Quantistica", provided by Prof. P. Tombesi, University of Camerino, Camerino (MC), Italy.
Feb 2011	Tutor for the Mathematics Olimpics, "Strategie e tecniche per soluzioni di problemi di fisica", University of Camerino, Camerino (MC), Italy.
Dec 2010	Lectures for the course of "Meccanica Quantistica", provided by Prof. P. Tombesi, University of Camerino, Camerino (MC), Italy.
Apr – May 2009	Lectures as tutor of physics for undergraduate students in "Chimica e Scienze Geologiche", in collaboration with Prof. S. Simonucci, and Biologia e "Scienze della Natura e dell'Ambiente", in collaboration with Prof. A. Di Cicco , University of Camerino, Camerino (MC), Italy.
2006-2008	Lectures on "Quantum Protocols" within the course of Quantum Mechanics held by Prof. P. Tombesi at the University of Camerino and on "Quantum Information" with Prof. S. Mancini.
2006, 2007	Physics Lectures within the program "AGEPROF" for "Corsi Speciali Abilitanti" (D.M. 85 del 18.11.2005).
Other achievements	Author and Prize Winner of the regional competitions "StartCup 2008 Perugia-Camerino" (20 K€) and "Innovative ideas for industry" (40 K€), which led to the foundation of the company "CriptoCam", spinoff of the University of Camerino.
	Member and Contributor of the European Telecommunications Standards Institute (ETSI) Industry Standardization Group (ISG) for the standardization of QKD. Current rapporteur for the work item about QKD Security Proofs.
	Removed for anonymity reasons.
Driving licence	A and B type driving licences

Publications

1. Paraïso, T. K., De Marco, I., Roger, T., Marangon, D. G., Dynes, J. F., Lucamarini, M., Yuan, Z. L., Shields, A. J. "High Bit-Rate Quantum Communication Chips", in Optical Fiber Communication Conference (OFC) 2019, OSA Technical Digest (Optical Society of America, 2019), paper Th1J.4; https://doi.org/10.1364/OFC.2019.Th1J.4
2. Paraiso, T. K., Roger, T., De Marco, I., Marangon, D. G., Sanzaro, M., Dynes, J., Lucamarini, M., Yuan, Z. L., Shields, A. J., "On-chip modulator-free optical transmitter for quantum and classical communications", Proc. SPIE 10921, Integrated Optics: Devices, Materials, and Technologies XXIII 109210U, (4 March 2019); https://doi.org/10.1117/12.2516242
3. Minder, M., Pittaluga, M., Roberts, G. L., Lucamarini, M., Dynes, J. F., Yuan, Z. L., Shields, A. J. Experimental quantum key distribution beyond the repeaterless secret key capacity, Nature Photonics 13, pp. 334-338 (2019). https://doi.org/10.1038/s41566-019-0377-7
4. Lucamarini, M., Viewpoint: Record Distance for Quantum Cryptography, Physics 11, 111 (5 Nov 2018). https://physics.aps.org/articles/v11/111

5. Lucamarini, M., Ward, M. B., Yuan, Z. L., Shields, A. J. *et al.* Implementation Security of Quantum Cryptography. ETSI White Paper No. 27, ISBN No. 979-10-92620-21-4 (July 2018). https://www.etsi.org/images/files/ETSIWhitePapers/etsi_wp27_qkd_imp_sec_FINAL.pdf
6. Roberts, G.L., Pittaluga, M., Minder, M., Lucamarini, M., Dynes, J.F., Yuan, Z.L., Shields, A.J. Patterning-effect mitigating intensity modulator for secure decoy-state quantum key distribution (2018) Optics Letters, 43 (20), pp. 5110-5113. DOI: 10.1364/OL.43.005110
7. Dynes, J.F., Lucamarini, M., Patel, K.A., Sharpe, A.W., Ward, M.B., Yuan, Z.L., Shields, A.J. Testing the photon-number statistics of a quantum key distribution light source (2018) Optics Express, 26 (18), pp. 22733-22749. DOI: 10.1364/OE.26.022733
8. Marangon, D.G., Plews, A., Lucamarini, M., Dynes, J.F., Sharpe, A.W., Yuan, Z., Shields, A.J. Long-Term Test of a Fast and Compact Quantum Random Number Generator (2018) Journal of Lightwave Technology, 36 (17), pp. 3778-3784. DOI: 10.1109/JLT.2018.2841773
9. Roberts, G.L., Lucamarini, M., Dynes, J.F., Savory, S.J., Yuan, Z.L., Shields, A.J. A direct GHz-clocked phase and intensity modulated transmitter applied to quantum key distribution (2018) Quantum Science and Technology, 3 (4), art. no. 045010. DOI: 10.1088/2058-9565/aad9bd
10. Koehler-Sidki, A., Lucamarini, M., Dynes, J.F., Roberts, G.L., Sharpe, A.W., Yuan, Z., Shields, A.J. Intensity modulation as a preemptive measure against blinding of single-photon detectors based on self-differencing cancellation (2018) Physical Review A, 98 (2), art. no. 022327. DOI: 10.1103/PhysRevA.98.022327
11. Yuan, Z., Plews, A., Takahashi, R., Doi, K., Tam, W., Sharpe, A., Dixon, A., Lavelle, E., Dynes, J., Murakami, A., Kujiraoka, M., Lucamarini, M., Tanizawa, Y., Sato, H., Shields, A.J. 10-Mb/s Quantum Key Distribution (2018) Journal of Lightwave Technology, 36 (16), pp. 3427-3433. DOI: 10.1109/JLT.2018.2843136
12. Martinez, A., Frohlich, B., Dynes, J.F., Sharpe, A.W., Tam, W., Plews, A., Lucamarini, M., Yuan, Z., Shields, A.J. Birefringent Interferometry for Quantum Key Distribution (2018) 2018 Conf. on Lasers and Electro-Optics, CLEO 2018 - Proceedings, art. no. 8426759. PUBLISHER: Inst. of Electrical and Electronics Engineers Inc. ISBN: 978-194358042-2
13. Martinez, A., Fröhlich, B., Dynes, J.F., Sharpe, A.W., Tam, W., Plews, A., Lucamarini, M., Yuan, Z., Shields, A.J. Quantum key distribution using in-line highly birefringent interferometers (2018) Applied Physics Letters, 113 (3), art. no. 031107. DOI: 10.1063/1.5036827
14. Lucamarini, M., Yuan, Z.L., Dynes, J.F., Shields, A.J. Overcoming the rate-distance limit of quantum key distribution without quantum repeaters (2018) Nature, 557 (7705), pp. 400-403. DOI: 10.1038/s41586-018-0066-6
15. Koehler-Sidki, A., Dynes, J.F., Lucamarini, M., Roberts, G.L., Sharpe, A.W., Yuan, Z.L., Shields, A.J. Best-Practice Criteria for Practical Security of Self-Differencing Avalanche Photodiode Detectors in Quantum Key Distribution (2018) Physical Review Applied, 9 (4), art. no. 044027. DOI: 10.1103/PhysRevApplied.9.044027
16. Roberts, G.L., Lucamarini, M., Dynes, J.F., Savory, S.J., Yuan, Z., Shields, A.J. Manipulating photon coherence to enhance the security of distributed phase reference quantum key distribution (2017) Applied Physics Letters, 111 (26), art. no. 261106. DOI: 10.1063/1.5004488
17. Roberts, G.L., Lucamarini, M., Yuan, Z.L., Dynes, J.F., Comandar, L.C., Sharpe, A.W., Shields, A.J., Curty, M., Puthoor, I.V., Andersson, E. Experimental measurement-device-independent quantum digital signatures (2017) Nature Communications, 8 (1), art. no. 1098. DOI: 10.1038/s41467-017-01245-5
18. Dixon, A.R., Dynes, J.F., Lucamarini, M., Fröhlich, B., Sharpe, A.W., Plews, A., Tam, W., Yuan, Z.L., Tanizawa, Y., Sato, H., Kawamura, S., Fujiwara, M., Sasaki, M., Shields, A.J. Quantum key distribution with hacking countermeasures and long term field trial (2017) Scientific Reports, 7 (1), art. no. 1978. DOI: 10.1038/s41598-017-01884-0
19. Roberts, G.L., Lucamarini, M., Dynes, J.F., Savory, S.J., Yuan, Z., Shields, A.J. Directly intensity-modulated quantum key distribution (2017) 2017 Conference on Lasers and Electro-Optics, CLEO 2017 - Proceedings, 2017-January, pp. 1-2. DOI: 10.1364/CLEO_QELS.2017.FTu4F.7
20. Roberts, G.L., Lucamarini, M., Dynes, J.F., Savory, S.J., Yuan, Z.L., Shields, A.J. Modulator-Free Coherent-One-Way Quantum Key Distribution (2017) Laser and Photonics Reviews, 11 (4), art. no. 1700067. DOI: 10.1002/lpor.201700067
21. Fröhlich, B., Lucamarini, M., Dynes, J.F., Comandar, L.C., Tam, W.W.-S., Plews, A., Sharpe, A.W., Yuan, Z., Shields, A.J. Long-distance quantum key distribution secure against coherent attacks (2017) Optica, 4 (1), pp. 163-167. DOI: 10.1364/OPTICA.4.000163
22. Roberts, G.L., Lucamarini, M., Dynes, J.F., Savory, S.J., Yuan, Z., Shields, A.J. Directly intensity-modulated quantum key distribution (2017) Optics InfoBase Conference Papers, Part F42-CLEO_QELS 2017, 2. DOI: 10.1364/CLEO_QELS.2017.FTu4F.7
23. Koehler-Sidki, A., Dynes, J.F., Lucamarini, M., Roberts, G.L., Sharpe, A.W., Savory, S.J., Yuan, Z., Shields, A.J. Setting best practice criteria for self-differencing avalanche photodiodes in quantum key distribution (2017) Proceedings of SPIE - The International Society for Optical Engineering, 10442, art. no. 104420L. DOI: 10.1117/12.2275675

24. Dynes, J.F., Tam, W.W.-S., Plews, A., Fröhlich, B., Sharpe, A.W., Lucamarini, M., Yuan, Z., Radig, C., Straw, A., Edwards, T., Shields, A.J. Ultra-high bandwidth quantum secured data transmission (2016) Scientific Reports, 6, art. no. 35149. DOI: 10.1038/srep35149
25. Comandar, L.C., Lucamarini, M., Fröhlich, B., Dynes, J.F., Yuan, Z.L., Shields, A.J. Near perfect mode overlap between independently seeded, gain-switched lasers (2016) Optics Express, 24 (16), pp. 17849-17859. DOI: 10.1364/OE.24.017849
26. Yuan, Z.L., Fröhlich, B., Lucamarini, M., Roberts, G.L., Dynes, J.F., Shields, A.J. Directly phase-modulated light source (2016) Physical Review X, 6 (3), art. no. 031044. DOI: 10.1103/PhysRevX.6.031044
27. Vallone, G., Di Giuseppe, G., Mataloni, P., Villoresi, P., Lucamarini, M. Reply to "Comment on 'Device-independent entanglement-based Bennett 1992 protocol" (2016) Physical Review A, 93 (6), art. no. 066304. DOI: 10.1103/PhysRevA.93.066304
28. Tamaki, K., Curty, M., Lucamarini, M. Decoy-state quantum key distribution with a leaky source (2016) New Journal of Physics, 18 (6), art. no. 065008. DOI: 10.1088/1367-2630/18/6/065008
29. Comandar, L.C., Lucamarini, M., Fröhlich, B., Dynes, J.F., Sharpe, A.W., Tam, S.W.-B., Yuan, Z.L., Penty, R.V., Shields, A.J. Quantum key distribution without detector vulnerabilities using optically seeded lasers (2016) Nature Photonics, 10 (5), pp. 312-315. DOI: 10.1038/nphoton.2016.50
30. Dynes, J.F., Kindness, S.J., Tam, S.W.-B., Plews, A., Sharpe, A.W., Lucamarini, M., Fröhlich, B., Yuan, Z.L., Penty, R.V., Shields, A.J. Quantum key distribution over multicore fiber (2016) Optics Express, 24 (8), pp. 8081-8087. DOI: 10.1364/OE.24.008081
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32. Fröhlich, B., Dynes, J.F., Lucamarini, M., Sharpe, A.W., Tam, S.W.-B., Yuan, Z., Shields, A.J. Quantum secured gigabit optical access networks (2015) Scientific Reports, 5, art. no. 18121. DOI: 10.1038/srep18121
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Other papers

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Patents

#	Title	Publication number	Publication date
1	Quantum communication component, receiver and system	US2019013878 (A1)	10/01/2019
2	Light quantum communication system	JP2018137739 (A)	30/08/2018
3	String processor	JP2017215974 (A); JP6397966 (B2)	07/12/2017
4	Optical device, transmitter for quantum communication system, and quantum communication system	JP2017146592 (A); JP6430553 (B2)	24/08/2017
5	Communication system and method	JP2017130932 (A); JP6303034 (B2)	27/07/2017
6	A quantum communication system	GB2550263 (A)	15/11/2017
7	A quantum communication system	GB2550264 (A); GB2550264 (A9); GB2550264 (B)	15/11/2017
8	Interference system and interference method	JP2016042694 (A); JP6100846 (B2)	31/03/2016
9	System and method for intensity monitoring	US2016087718 (A1); US9853727 (B2)	24/03/2016
10	Random number generator	JP2016006629 (A); JP6072105 (B2)	14/01/2016
11	Optical device	JP2016001868 (A); JP5973022 (B2)	07/01/2016
12	Optical device	US2015304051 (A1); US9876580 (B2)	22/10/2015
13	An interference system and a method of fabricating an interference system	GB2540589 (A); GB2540589 (B)	25/01/2017
14	An optical device	GB2537821 (A); GB2537821 (B)	02/11/2016
15	An optical device	GB2525501 (A); GB2525501 (B)	28/10/2015
16	Qudits in two way deterministic quantum key distribution	MY153146 (A)	31/12/2014
17	An interference system and an interference method	GB2529228 (A); GB2529228 (B)	17/02/2016
18	Quantum cryptography system with error correction and privacy amplification	GB2503045 (A); GB2503045 (A9); GB2503045 (B)	18/12/2013
19	Description of the patent application entitled: quantum signals receiver with noise compensation, quantum cryptography communications system and method	WO2011033543 (A1)	24/03/2011
20	Endless polarization control using a feedback algorithm	WO2010134107 (A1)	25/11/2010
21	Random number generator based on homodyne detection with a phase randomized local oscillator	PN828268GB	Filed on: 25/06/2018
22	Stable high-speed generation of optical pulses with three or more different intensities including at least one low-contrast pair of intensities	PN828267GB	Filed on: 22/02/2018

Conferences

Removed for anonymity reasons

A taste of Press

Removed for anonymity reasons

CURRICULUM VITAE

Education (Academic-employment)

- **2014-January-2019 April**: Senior Research Fellow at National University of Singapore (NUS), Graphene Research Centre (GRC), Centre for Advanced 2D materials (Ca2dm), and Singapore Synchrotron Light Source (SSLS), Singapore.
- **2013 July-December:** Senior Research fellow at iit-istituto italiano di tecnologia, Italy
- **2011 July-2013 July**: Fixed term researcher at CNR Lecce, Italy.
- **2010 January-2011 June:** Scientist at Max Planck Institute, Halle-Salle, Germany.
- **2009:** Research fellow at Université de Montréal, Québéc, Canada.
- **2008:** Ph.D. in Physics at University College London and London Centre for Nanotechnology.

Ph.D. Thesis title: "Theoretical models of photo induced processes at surfaces of oxide nano-particles". Seven (7) scientific articles published and five (5) Conference contributions. Final Mark: Passed

PhD Thesis written during my Post doc at CNRS in Grenoble.

- **2007 February-2008 December:** Research fellow at Institut Néel, CNRS, Grenoble (France).
- **2003 September-2007 January:** Ph. D. student in Physics at University College London (UCL) & London Centre for Nanotechnology (LCN).

--2001-2003 (see industrial employment)--

- **1992-2000 September:** MSc. in Physics at "La Sapienza" University of Rome.

MSc Thesis title: "Coupling, propagation, and absorption of the energy of Ion Bernstein wave in Tokamak plasma." I developed my Thesis at FTU tokamak centre (EURATOM-ENEA) .

Industrial employment

2001-2003 Software Engineer consultant at Finmeccanica group ltd on behalf of S.I.A. ltd. Software-developer of *real-time* remote-control programs for the radio ships control. This software is currently working in the *"Pattugliatore"* naval ship class of the Italian navy. The programs are coded in C/C++ and Java.

Technological Skills

- **Developer**

FORTRAN 90/77: I am developer of Condensed Matter Density Functional and ab initio many body codes: **Hippo** Density matrix functional theory code, **DP-code** and **EXC code**: TDDFT and Bethe Salpeter Equation code, and **TurboMole** quantum chemistry code.

C/C++: Project developer of client-server remote controls and "drivers" for the Italian and Chinese Defence software.

Java: Project developer of client-server remote control and "drivers" for the management of the Nato Defence hardware. These codes were developed in multithreading.

Python: PyQt4, TensorFlow

- **User**
- **DFT: Abinit, Quantum Espresso**

  GW: Abinit, Yambo, BerkeleyGW

  TDDFT: DP-code, Yambo code, BerkeleyGW

  Bethe Salpeter Equation: DP-EXC, Yambo code, BerkeleyGW

  Quantum chemistry: Gaussian, Gamess, Crystal, TurboMole

  Reduced Density Matrix Functional Theory code: Hippo

Used operating systems: Good knowledge: UNIX; Linux; Windows 9x, NT, 2000, XP; MacOs.

Language skills

- ***English***: fluent

  Attended Course: University College London English course for foreigners: Intermediate
- ***French***: Advanced

  Attended Course: (diplôme d'études secondaires en formation générale A2 : LAN50714 (equivalent to an Advanced course)

  Final result : 75/100. Delivered by the *Ministère de l'Education, du Loisir et du Sport,*

Québec Canada)

- ***Italian***: mother tongue

Teaching skills:

Thermodynamics & Statistical Mechanics (Module 2230) Lecturer in the Department of Engineering at National University of Singapore (2016-2017)

Abilitazione nazionale Italiana SETTORE CONCORSUALE 02/B2 a professore fascia II. Valido fino al 2024.

Research Contribution

➔ **List of publications:**

1. D. Frigione et al., *Steady improved confinement in FTU high field plasmas sustained by deep pellet injection*. Nuclear Fusion, 41 (11): 1613-1618, 2001.
2. R. Cesario et al., *Reduction of the electron thermal conductivity produced by ion Bernstein waves on the Frascati tokamak*, Physics of Plasmas 8(11):4721(2001).
3. P.E. Trevisanutto, P.V. Sushko, A.L. Shluger, K.M. Beck, M. Henyk, A.G. Joly, and W.P. Hess, *A mechanism of photo-induced desorption of oxygen atoms from MgO nanocrystals*, Surf. Sci. 593:210, 2005.
4. W.P. Hess, A.G. Joly, K.M. Beck, M. Henyk, P.V. Sushko, P.E. Trevisanutto, and A.L. Shluger, *Laser control of desorption through selective surface excitation*, FEATURE ARTICLE. J. Phys. Chem. B 109:19563, 2005.
5. K.M. Beck, M. Henyk, C. Wang , P.E. Trevisanutto, P.V. Sushko, W.P. Hess, and A.L. Shluger, *Site-specific modification of oxide nanoclusters: Towards atomic-scale surface structuring*, Phys. Rev. B 74:45404, 2006.
6. A.G. Joly, M. Henyk, K.M. Beck, P.E. Trevisanutto, P.V. Sushko, W.P. Hess, and A.L. Shluger, *Probing electron transfer dynamics at MgO surfaces by Mg-atom desorption*, J. Phys. Chem. B 37:18093, 2006.
7. M. Müller, S. Stankic , O. Diwald, E. Knözinger , P.V. Sushko , P.E. Trevisanutto, and A.L. Shluger , *Effect of protons on the optical properties of oxide nanostructures*, J. Am. Chem. Soc. 129(41):12491, 2007.

8. K.M. Beck, A. G. Joly, M. Henyk, O. Diwald, S. Stankic, P.E. Trevisanutto, P.V. Sushko, A.L. Shluger, and W. P. Hess, *Energy and site selectivity in O-atom photodesorption from nanostructured MgO*. Surf. Sci. 602:1968, 2008.

9. P.E. Trevisanutto, C. Giorgetti, L. Reining, M. Ladisa, V. Olevano, *Ab initio GW ManyBody effects in graphene*, Phys. Rev. Lett. **101**, 226405 (2008)

10. P.E. Trevisanutto, P.V. Sushko, A.L. Shluger, K.M. Beck, A.G. Joly, M. Henyk, and W.P. Hess, *Excitation, ionization, and desorption: how sub-band-gap photons modify the electronic properties and atomic structure of oxide nanoparticles*, J. Phys. Chem. C 113(4):1274-1279 (2009).

11. P. E. Trevisanutto, M. Holzmann, M. Côté., V. Olevano *High-energy excitonic effects in graphite and graphene*: also in cond. Mat arXiv: 0909.1682. Phys. Rev. B 81, 121405(R) (2010).

12. S. Levesque, P. E. Trevisanutto, J. F. Laprade, M. Côté.. Ab initio study of Diketo-Pyrrole Polymers for photovoltaic applications, also in cond. Mat arXiv: 0911.0224v1.

13. T. Rangel, A. Ferretti, P. E. Trevisanutto, V. Olevano, G.-M. Rignanese. *Transport properties of molecular junctions from many-body perturbation theory*. ArXiv 1102.1880. Phys. Rev. B 84, 045426 (2011).

14. T. Rangel, D. Kecik, P. E. Trevisanutto, G.-M. Rignanese, H. Van Swygenhoven, and V. Olevano. *Band structure of gold from many-body perturbation theory*. Phys. Rev. B 86, 125125 (2012). also in arXiv: 1203.4508v1

15. A.Tanwar, E. Fabiano, P. E. Trevisanutto, L. Chiodo, F. Della Sala. *Accurate ionization potential of gold anionic clusters from density functional theory and many-body perturbation theory*. European Phys. Journal B 86, 161 (2013)

16. P. E. Trevisanutto, A. Terentjevs, L. A. Constantin, V. Olevano, and F. Della Sala. *Optical spectra of solids obtained by time-dependent density-functional theory with Jellium with Gap Model exchange-correlation kernel.* Phys. Rev. B 87, 205143 (2013). also in in arXiv: 1210.7149

17. E. Fabiano, P. E. Trevisanutto, A. Terentjevs, L. A. Constantin, *Generalized gradient approximation correlation energy functionals based on the uniform electron gas with gap model*. J. Chem. Theory and Computation 10 (5), 2016 (2014)

18. A. Terentjevs, P. E. Trevisanutto L. A. Constantin F. Della Sala. *First principles Time Dependent DFT calculations of the optical spectra for the β-SiC(001)/Al interface*. J. Phys.: Condens. Matter 26 (2014) 265006.

19. P.K. Gogoi, P. E. Trevisanutto, Ming Yang, I. Santoso, Teguh Citra Asmara, A. Terentjevs, Fabio Della Sala, Mark B. H. Breese, T. Venkatesan, Yuan Ping Feng, Kian Ping Loh, A. H. Castro Neto, A. Rusydi. *Graphene optical conductivity renormalization on $SrTiO_3$ due to Ti-3d orbitals mediated resonant excitonic effects.* Phys. Rev. B 91 , 035424 (2015)

20. A. Ziletti, A. Carvalho, P.E. Trevisanutto, D.K. Campbell, D.F. Coker, and A.H. Castro Neto. *Phosphorene oxides: bandgap engineering of phosphorene by oxidation.* Phys. Rev. B. 91, 0850407 (2015) Also in ArXiv:1410.3906v1

21. Yeo, L. H. and Srivastava, A. and Majidi, M. A. and Sutarto, R. and He, F. and Poh, S. M. and Diao, C. and Yu, X. and Motapothula, M. and Saha, S. and Ojha, S. and Kanjilal, D. and Trevisanutto, P. E. and Breese, M. B. H. and Venkatesan, T. and Rusydi, A. *Anomalous spectral-weight transfers unraveling oxygen screening and electronic correlations in the insulator-metal transition of VO_2.* Phys. Rev. B 91, 081112(R) (2015)

22. P.K. Gogoi, L. Sponza, D. Schmidt, Teguh Citra Asmara, Caozheng Diao, Jason Lim, Sock M. Poh, P. E. Trevisanutto, V. Olevano, A. Rusydi. *Anomalous excitons and screenings unveiling strong electronic correlations in Sr $Ti_{1-x}Nb_xO_3$.* Phys. Rev. B 92 035119 (2015)

23. P.E. Trevisanutto and M. Millettari. *Hedin Equations in resonant Microcavities.* Phys. Rev. B 92 (23), 235303 (2015)

24. Yong Zhihua, Paolo E. Trevisanutto, L. Chiodo,Iman Santoso, Arkajit R. Barman, Teguh Citra Asmara, Sankar Dhar, A. Terentjevs, F. Della Sala, V. Olevano, Michael Rübhausen, T. Venkatesan, Andrivo Rusydi. *Emerging giant resonant exciton induced by Ta doping in anatase TiO2: a correlation effect.* Physical Review B 93 (20), 205118 (2016)

25. P.E. Trevisanutto and G. Vignale. Ab initio electronic structure of quasi two-dimensional materials: a ``native" gaussian--plane wave approach. *The Journal of chemical physics* 144 (20), 204122 (2016)

26. L.C. Gomes, P.E. Trevisanutto, A. Carvalho, A.S. Rodin, A.H. Castro-Neto. *Strongly bound Mott-Wannier Excitons in GeS and GeSe monolayers.* arXiv preprint arXiv:1607.07564. Phys. Rev. B 94 (15), 155428 (2016)

27. A. Marmodoro, A. Ernst, S. Ostanin, L.Sandratskii, P.E. Trevisanutto, N. Lathiotakis, J.B. Staunton. *Short-range ordering effects on the electronic Bloch's spectral function of real materials in the non local coherent potential approximation.* Physical Review B 94 (22), 224205 (2016)

28. Teguh Citra Asmara, Yongliang Zhao, Muhammad Aziz Majidi, Christopher T. Nelson, Mary C. Scott, Yao Cai, Dongyang Wan, Daniel Schmidt, Ming Yang, Paolo E. Trevisanutto, Mallikarjuna R. Motapothula, Mark B.H. Breese, Matthew Sherburne, Mark Asta, Andrew

Minor, T. Venkatesan, Andrivo Rusydi. *Tunable and low-loss correlated plasmons in Mott-like insulating oxides.* Nature communications 8, 15271 (2017).

29. Xiao Chi, Zhen Huang, Teguh C. Asmara, Kun Han, Xinmao Yin, Xiaojiang Yu, Caozheng Diao, Ming Yang, Daniel Schmidt, Ping Yang, Paolo E. Trevisanutto, T. J. Whitcher, T. Venkatesan, Mark B. H. Breese, Ariando, and Andrivo Rusydi. *Large Enhancement of 2D Electron Gases Mobility Induced by Interfacial Localized Electron Screening Effect.* Adv.Mater. (2018), 30, 1707428
30. Tao Zhu, Paolo E Trevisanutto, Teguh Citra Asmara, Lei Xu, Yuan Ping Feng, Andrivo Rusydi. *Generation of multiple plasmons in strontium niobates mediated by local field effects* . Phys. Rev. B 98, 235115 (2018)
31. Mirco Milletarí, Thiparat Chotibut, Paolo E Trevisanutto. *Expectation propagation: a probabilistic view of Deep Feed Forward Networks.* Submitted to Neural Networks.also arXiv preprint arXiv:1805.08786

➔ **Conference contributions (Selected list):**

- P.E. Trevisanutto, A. Cardinali, N. Castaldo. "Evolution of the WKB amplitude of the ion Bernstein wave electric field along the wave propagation": poster presentation 9th European Nuclear Fusion theory conference, Helsinborg (Denmark) in October 2001
- P.E. Trevisanutto, P.V. Sushko, A.L. Shluger. "A Bi-exciton mechanism of photo-induced desorption from MgO": poster presentation. NanoExc 2004 Workshop Acquafredda di Maratea Italy. September 2004
- P.E. Trevisanutto, P.V. Sushko, A.L. Shluger. "Mechanisms of photo-induced desorption from MgO nano-particles": poster presentation 10th DIET conference Susono, Japan. November 2004
- P.E. Trevisanutto, P.V. Sushko, A.L. Shluger "Mechanisms of photo-induced desorption from MgO nano-particles": poster presentation. Psik2005 Workshop. September 2005
- P.E. Trevisanutto, P.V. Sushko, A.L. Shluger "Mechanisms of photo-induced processes in MgO nano-particles": oral presentation. 10th Eurodim Conference. July 2006
- P.E. Trevisanutto, P.V. Sushko, A.L. Shluger "Mechanisms of photo-induced processes in MgO nano-particles": oral presentation. ECOSS 24 Conference. September 2006
- P.E. Trevisanutto, C. Giorgetti, L. Reining, M. Ladisa, V. Olevano *Ab initio* dynamical correlation effects in graphene, oral presentation. Nanoquanta-ETSF 5th young research meeting, Modena 2008

- P.E. Trevisanutto, C. Giorgetti, L. Reining, M. Ladisa, V. Olevano *Ab initio* dynamical correlation effects in graphene, oral presentation. CMD 22 European Physical Society, Rome 2008.
- P.E. Trevisanutto, C. Giorgetti, L. Reining, M. Ladisa, V. Olevano *Ab initio* dynamical correlation effects in graphene, oral presentation. 13th Nanoquanta-Etsf Workshop on Electronic Excitations, Pugnochiuso 2008
- P. E. Trevisanutto, A. Terentjevs, L. A. Constantin, V. Olevano, and F. Della Sala. *Optical spectra of solids obtained by time-dependent density-functional theory with Jellium with Gap Model exchange-correlation kernel.* Gordon Research Seminars oral presentation, Biddeford 2013.
- Workshop on Optical Conductivity of Functional Materials on the 9-11th of June 2014 at Institut Teknologi Bandung (ITB). Invited Guest Lecturer.
- December 11-15th 2017. 3rd International Conference on ICON-2DMAT 2017: Invited talk.

INFORMAZIONI PERSONALI

Alessio Troiani

FORMAZIONE

Ottobre 2012 — **Dottorato in Matematica (PhD)**
Università di Leiden (Paesi Bassi) Titolo della tesi: "Metastability for low-temperature Kawasaki dynamics with two types of particles".
Relatori: Prof. Dr. F. den Hollander (Università di Leiden) e Dr. F. R. Nardi (TU Eindhoven).

Ottobre 2007 — **Laurea Specialistica** *cum laude* in Ingegneria Gestionale
Università degli Studi di Roma "Tor Vergata"
Relatore: Prof. B. Scoppola.

Luglio 2007 – Ottobre 2007 — **Visiting Student** (Special Focus Year on Discrete Random Systems)
Center for Discrete Mathematics and Theoretical Computer Science (DIMACS) – Rutgers, The State University of New Jersey
Supervisore: Prof. Dr. J. L. Lebowitz.

Ottobre 2004 — **Laurea** *cum laude* in Ingegneria Gestionale
Università degli Studi di Roma "Tor Vergata"
Relatore: Prof. B. Scoppola.

ATTIVITÀ ACCADEMICA

Maggio 2018 – Maggio 2019 — **Assegnista di ricerca**
Dipartimento di Matematica – Università degli Studi di Padova
Tema di ricerca: Statistical Study of Gravitational Systems
Supervisor: Prof.ssa Gabriella Pinzari

Maggio 2017 – Aprile 2018 — **Assegnista di ricerca**
Dipartimento di Matematica – Università degli Studi di Firenze
Tema di ricerca: Dinamiche stocastiche parallele e applicazioni alla meccanica statistica
Supervisor: Prof.ssa Francesca R. Nardi

Novembre 2015 – Novembre 2016 — **Assegnista di ricerca**
Dipartimento di Matematica – Università degli Studi di Roma "Tor Vergata"
Tema di ricerca: Dinamiche stocastiche parallelle e calcolo su GPU
Supervisor Prof. Benedetto Scoppola

ATTIVITÀ DI INSEGNAMENTO

Febbraio 2019 – Maggio 2019
Docente a contratto
Corso "Statistics" – LUISS Guido Carli

Settembre 2018 – Dicembre 2018
Docente a contratto
Corso "Elementary probability"– LUISS Guido Carli

Febbraio 2018 – Maggio 2018
Docente a contratto
Corso "Statistics" – LUISS Guido Carli

Settembre 2017 – Dicembre 2017
Docente a contratto
Corso "Elementary probability"– LUISS Guido Carli

Settembre 2016 – Dicembre 2016
Assistente alla didattica
Corso "Elementary probability"– LUISS Guido Carli

Marzo 2016 – Giugno 2016
Assistente alla didattica
Corso "Calcolo delle probabilità" – Dipartimento di Matematica – Università degli studi di Roma "Tre"

Gennaio 2011 – Giugno 2011
Assistente alla didattica
Corso "Stochastic Processes" – "Dutch master's degree program in mathematics" – Paesi Bassi.

Settembre 2009 – Gennaio 2012
Assistente alla didattica
Corso "Introductory Statistics" (anni accademci 2009/10 - 2010/11 - 2011/12) – Facoltà di Scienze – Università di Leiden – Paesi Bassi

PUBBLICAZIONI

Shaken dynamics for the 2d ising model, arXiv:1904.06257 (with V. Apollonio, R. D'Autilia, B. Scoppola and E. Scoppola)

Gaussian Mean Fields Lattice gas, *Journal of Statistical Physics* (2018), 170:1161, https://doi.org/10.1007/s10955-018-1984-2, (with B. Scoppola)

The blockage problem, *Bulletin of the Institute of Mathematics Academia Sinica (New Series)*, 8(1), 49–72, 2013, ISSN: 2304-7895 [online] (with O. Costin, J. L. Lebowitz and E. R. Speer).

Metastability for Kawasaki dynamics with two types of particles, PhD Thesis, 2012, ISBN 9789461914644, handle: http://hdl.handle.net/1887/20065

Metastability for Kawasaki dynamics with two types of particles: critical droplets, *Journal of Statistical Physics*, 149, 1013–1057, 2012, https://doi.org/10.1007/s10955-012-0637-0 (with F. den Hollander and F. R. Nardi).

Metastability for Kawasaki dynamics with two types of particles: stable/metastable configurations and communication heights, *Journal of Statistical Physics*, 145, 1423–1457, 2011, https://doi.org/10.1007/s10955-011-0370-0 (with F. den Hollander and F. R. Nardi).

Metastability for Kawasaki dynamics at low temperature with two types of particles, *Electronic Journal of Probability*, 17(2), 1–26, 2012, doi:10.1214/EJP.v17-1693 (with F. den Hollander and F. R. Nardi).

SELECTED TALKS

Marzo 2019	Mathematical Physics and Related Subjects Seminar, Università di Padova (Italia)
Maggio 2018	Probability Seminar, Università di Leiden (Paesi Bassi).
Marzo 2012	Mark Kac Seminar on Stochastics and Physics, Utrecht (Paesi Bassi).
Luglio 2011	Cornell Probability Summer School, Ithaca (USA).
Maggio 2011	Oberseminar Stochastics, Università di Bonn (Germania).
Maggio 2010	Probability Seminar, Università di Leiden (Paesi Bassi).

ATTIVITÀ NON ACCADEMICA

Settembre 2014 – Dicembre 2018

Attività di consulenza e formazione su
- Salute e sicurezza nei luoghi di lavoro
- Igiene degli alimenti
- Quality management

Ottobre 2012 – Giugno 2014

Software Engineer
Team di Studi Statistici (dipartimento di revenue management)
Amadeus (Sophia Antipolis - Francia)

Febbraio 2008 – Aprile 2008

Business Analyst
Accenture Italia S.p.a.

COMPETENZE PERSONALI

MADRELINGUA Italiano

ALTRE LINGUE

	Comprensione		Parlato		Produzione scritta
	Ascolto	Lettura	Interazione	Produzione orale	
Inglese	C2	C2	C2	C2	C2
Francese	B1	C1	B2	B1	B1
Olandese	A2	A2	A2	A2	A2

A1, A2: Utente base; B1, B2: Utente autonomo; C1, C2: Utente avanzato

LINGUAGGI DI PROGRAMMAZIONE Python, Julia, C/C++, Fortran, R, CUDA, SQL, LaTeX

ALTRO

Gennaio 2015 – presente: Membro dell'Ordine Provinciale degli Ingegneri di Roma

Settembre 1989 – Luglio 2008: Nuotatore agonista (Nazionale Juniores; Campione Italiano Giovanile; Medagliato Campionati Nazionali)

Trattamento dei dati personali autorizzato ai sensi del D. Lgs. 196/2003 e del Regolamento UE 2016/679.