Consiglio Nazionale delle Ricerche
Istituto Nanoscienze

Current position

From 01.04.2021

Postdoctoral Researcher at the S3 Center, Istituto Nanoscienze CNR of Modena (Italy) under the supervision of Dr. Claudia Cardoso to work on the development and application of computational methods at the Many Body Perturbation Theory level by means of the Yambo code to study optical properties of defective Titanium Dioxide.

Education

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

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**.

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**.

Previous Research experience

From 14.09.2015

to 29.02.2021: Postdoctoral Research Associate at King's College London, London (U.K.), under the supervision of Prof. Mark van Shilfgaarde and Dr. Nicola Bonini to work on the evaluation of 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.

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.

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 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 1.06.2009

to 31.05.2010: winner of the scholarship at the National Nanotechnology Laboratory (NNL), Lecce, Italy, CNR-INFM, Unità Operativa di Lecce, to carry out studies and research for the ERC project, Development of Density Functional Theory methods for Organic Metal Interaction (DEDOM) for the thematic *Simulation of organic molecules on metallic substrate*.

Teaching experience

15.05.2019: *Electron-phonon in Quasiparticle Self-consistent GW* course during the *QUESTAAL Summer School 2019* held from 13 to 17 May, Darensbury Laboratory, U.K.

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.)

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

Scientific Societies

- Topic editor for **Materials** (see https://www.mdpi.com/journal/materials/topic_editors

- Member of **American Physical Society (APS)**

Skills

Computer

Operating systems:

- Linux (good)

Quantum-chemistry softwares:

- QUESTAAL (good, developer; see https://www.questaal.org/about/developers/)
- YAMBO (good, developer)
- TURBOMOLE (good, developer)
- ABINIT (good,developer)
- QUANTUM ESPRESSO (good)

Programming languages and scripts:

- Fortran (good)
- C (good)
- Shell scripting (good)
- Python (beginner)
- Parallel programming within MPI (good)
- Experience in using SVN with TURBOMOLE and GitHub/GitLab for the remaining softwares
- Exsperience in using highly parallel scientific libraries as Scalapack and SLEPc in YAMBO

Languages

- Italian (mother tongue)
- English (fluent)

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Research interests

Postdoctoral Research at the S3 Center, Istituto Nanoscienze CNR of Modena (from 01/04/2021 to present)

In this third postdoctoral experience my research interest is focused on the accurate characterization of anisotropic d-d excitations from surface-localized band-gap states in reduced rutile TiO_2(110), as reported in state selective studies using two-photon photoemission (2PPE) spectrosscopy. The computational studies are performed within a many-body perturbation theory (MBPT) framework, where the GW method combined with the solution of the Bethe-Salpeter equation (BSE) provides a powerful but computationally demanding tool for describing optical excitations of condensed matter systems from first principles. A further complication in the theoretical study occurs in the modeling of surface localized BGS, which requires a large supercell with at least four Ti layers in order to describe the electron self-trapping mechanism underlying the localization of a polaronic charge in the semi-infinite TiO_2 surface. Therefore, the complexity of the MBPT theoretical framework combined with the size of the slabs, required to model polaronic states, make the calculations very computationally demanding and possible only with HPC resources. I am making use of the Quantum-Espresso and the Yambo codes. The Yambo code is a flagship code of the EU MaX "Materials Science at the Exascale" Centre of Excellence (http://www.max-centre.eu/), and successfully ported to GPUs. Thanks to this experience I had chance to gain experience in using data software libraries as **HDF5** and **NetCDF** and highly parallel scientific libraries as **Scalapack**, **SLEPc**. I am also working in interfacing the Yambo code with the **NVIDIA Multi-process cuSOLVERMp** library, a high-performance, distributed-memory, GPU-accelerated library that provides tools for the solution of dense linear systems and eigenvalue problems that make use of ScaLAPACK-like C functionalities.

Postdoctoral Research Associate at King's College London (from 14/09/2015 to 28/02/2021)

In this second postdoctoral experience my research interest was focused on the evaluation of the phonon dispersion curves and of the electron-phonon interaction 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 is 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. The electron-phonon coupling (which can be a challenge in Density Functional Theory because of the implicit approximation of the inverse dielectric matrix)

has been evaluated in the Hedin-Lundqvist formalism at a many-body level of theory. The static inverse dielectric matrix has been evaluated both in the RPA approximation and by adding ladder diagrams through the solution of the Bethe-Salpeter equation. The evaluation of the electron-phonon matrix elements requires an

interpolation over a fine mesh of phonon wave vectors (which can be of the order 130x130x130 in case of diamond), therefore making the calculations very computationally demanding. The code has then been massively parallelized to make possible electron-phonon calculations with HPC resources . My interests at King's College London were also focused on the study of thermoelectric and structural properties of thermoelectric material. Of interest is the implementation in the QUESTAAL package of a relativistic Full Potential Linear Muffin-Tin (FP-LMTO) Orbital treatment of the magnetic quantum number that has been used to model core hole relaxation in X-Ray Photoelectron Spectroscopy (XPS) spectra because of the chemical environment. Core binding energies were then computed within the Δ Self-Consistent Field (ΔSCF) approximation at the DFT level of theory.

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 the Random Phase Approximation (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 was a bottleneck in the evaluation of the xc energy beyond the RPA approximation and a parallelization has been required.

Scholarship (from 01/06/2009 to 31/05/2010), Ph.D. (from 17/06/2010 to 17/06/2013) and the occasional collaboration contracts

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).

Role in international projects

I have been co-author of the "*Report on the simulations performed and scientific outlook*", deliverable number D6.3 for the project "***Materials Design at the Exascale***" (**MaX**), an European Centre of Excellence in materials modelling, simulations and design, 01/12/2018 – 30/09/2022.

Allocation history in PRACE, national calls, as well as international programs for computational resources

1) ISCRA Class C Project with title "Role of the hydroxyl defects in the formation of the deep band-gap state in TiO_2(110) surface" (TiO2-HYD) with 57600 CPU/hours on Marconi 100, 17/11/2021 - 17/08/2022
2) ISCRA Class B Project with title "MAny-body perturbation Theory description of anisotropic d-d Transitions in defected rutile TiO_2(110) Surfaces" (MATTIOS; ref. code: HP10BJM1QM) with 728000 CPU/hours on Marconi 100, 14/04/2022 - 14/06/2023
3) EuroHPC Regular Access call with title "Defect-induced fingerprints in Nb-doped TiO_2 Rutile Optical spectra within a Many-body perturbation theory formalism" (DNROM; EU2022R03-232) with 1500000 CPU/hours on Karolina GPU, 08/03/2023 - 07/03/2024

Publications

1) K. Chen, C. Di Paola, **S. Laricchia**, M. J. Reece, C. Weber, E. McCabe, I. Abrahams, and N. Bonini, Structural and Electronic Evolution in the Cu_3SbS_4-Cu_3SnS_4 Solid Solution, *J. Mater. Chem. C* **8**, 11508 (2020).
2) C. Di Paola, F. Macheda, **S. Laricchia**, C. Weber, N. Bonini, First-principle study of electronic transport and structural properties of $Cu_{12}Sb_4S_{13}$ in its high-temperature phase, *Phys. Rev. Research* **2**, 033055 (2020).

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

4) 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).

5) 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).

6) **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).

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

8) 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).

9) **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).

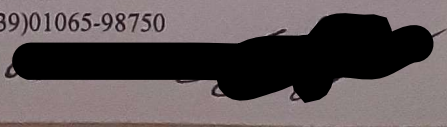
10) L. Chiodo, A. Massaro, **S. Laricchia**, F. Della Sala, R. Cingolani, M. Salazar, A. H. Romero and A. Rubio, Characterization of TiO_2 atomic crystals for nanocomposite materials oriented to optoelectronics, *Optical and Quantum Electronics.* **44**, 291 (2012).

11) **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).*

12) **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).

13) 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).

14) **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).



15) 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).

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

17) 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).

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

Invited talks

1) 11/03/2019 seminar hosted by Stephan Lany, National Renewable Energy Laboratory, Golden, Colorado, USA.

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

3) 19/11/2012 – 20/11/2012 Giulia Galli's group, University of California, Davis, California, USA.

Contributions and attendance to conferences

1) ***TALK:*** **S. Laricchia**, A. Ferretti, D. Varsano, C. Cardoso, A combined G_0W_0/BSE scheme of characterizing surface polaron photoexcitations in hydroxylated rutile TiO_2(110), *DPG Spring Meeting of the Condensed Matter Section (SKM)*, 26-31 March 2023, Dresden (Germany)

2) ***POSTER:*** **S. Laricchia**, A. Ferretti, D. Varsano, C. Cardoso, A. Selloni, A combined G_0W_0/BSE scheme of characterizing surface polaron photoexcitations in hydroxylated rutile TiO_2(110), *21th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods*, 11-13 January 2023, ICTP, Trieste (Italy)

3) ***TALK:*** **S. Laricchia**, N. Bonini, M. van Schilfgaarde, Electron-phonon coupling within Quasiparticle Self-consistent GW. *European Theoretical Spectroscopy Facility (ETSF),* 16-20 September 2019, Jena, Germany

4) ***TALK:*** **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 (Massachusetts; U.S.A.)

5) ***ATTENDANCE:*** Workshop on electron-phonon interaction, 22-24 May 2018, in Louvain-la-Neuve, Belgium. http://elphon.etsf.eu/list-participants

6) ***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/

7) ***ATTENDANCE:*** American Physical Society (APS) March meeting, 02-06 March 2015, San Antonio (Texas; U.S.A.)

8) ***POSTER:*** **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

9) ***POSTER:*** **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

Training schools

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.

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

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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.

Consapevole che, ai sensi dell'art.76 del DPR 445/2000, le dichiarazioni mendaci, la falsità negli atti e l'uso di atti falsi sono punite ai sensi del Codice penale e delle leggi speciali vigenti in materia, dichiara sotto la propria responsabilità:

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1) Datare e sottoscrivere tutte le pagine che compongono la dichiarazione.

2) Allegare alla dichiarazione la fotocopia di un documento di identità personale, in corso di validità.

3) Le informazioni fornite con la dichiarazione sostitutiva devono essere identificate correttamente con i singoli elementi di riferimento (esempio: data, protocollo, titolo pubblicazione ecc...).

4) Il CNR, ai sensi dell'art. 71 e per gli effetti degli artt. 75 e 76 del D.P.R. 445 del 28/12/2000 e successive modifiche ed integrazioni, effettua il controllo sulla veridicità delle dichiarazioni sostitutive.

5) La normativa sulle dichiarazioni sostitutive si applica ai cittadini italiani e dell'Unione Europea.

6) I cittadini di Stati non appartenenti all'Unione, regolarmente soggiornanti in Italia, possono utilizzare le dichiarazioni sostitutive di cui agli artt. 46 e 47 del D.P.R. 445 del 28.12.2000 limitatamente agli stati, alla qualità personali e ai fatti certificabili o attestabili da parte di soggetti pubblici italiani, fatte salve le speciali disposizioni contenute nelle leggi e nei regolamenti concernenti la disciplina dell'immigrazione e la condizione dello straniero.
Al di fuori dei casi sopradetti, i cittadini di Stati non appartenenti all'Unione autorizzati a soggiornare nel territorio dello Stato possono utilizzare le dichiarazioni sostitutive nei casi in cui la produzione delle stesse avvenga in applicazione di convenzioni internazionali fra l'Italia e il Paese di provenienza del dichiarante.

Cognome LARICCHIA

Nome SAVIO

nato il 10/03/1982

(atto n. 24 P. 2 S. A 1982)

a TRIGGIANO (BA)

Cittadinanza ITALIANA

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Firma del titolare

Il Adelfia 19/04/2019

IL SINDACO

Impronta del dito indice sinistro

IL SINDACO
Dott. Giuseppe Cosola