PERSONAL INFORMATION:

- First name, Family name : Fabio Della Sala

CURRENT POSITION(S):

- **Research Director (*Dirigente di Ricerca*)** at **Institute for Microelectronic and Microsystems (CNR-IMM),** University of Salento, Lecce.
- Associated Researcher at *Istituto Italiano di Tecnologia* (IIT), Center for Biomolecular Nanotechnologies (CBN), Arnesano (Lecce).

LINKS:

- Google Schoolar: https://scholar.google.it/citations?user=KR6o20AAAAAJ&hl=it
- ORCID: https://orcid.org/0000-0003-0940-8830
- CNR-IMM https://www.imm.cnr.it/users/fabiods
- CBN-IIT https://cbn.iit.it/research/researchareas/density-functional-theory

EDUCATION:

- *May 1998:* **Graduated in Electronic Engineering** *magna cum laude*, at University of Rome "Tor Vergata".
- *Dec. 2001:* **Ph. D. in Microelectronics and Telecommunications Engineering** at University of Rome "Tor Vergata".

PREVIOUS POSITIONS AND RESEARCH EXPERIENCES:

- *Mar.-Aug. 2000:* **Visiting scientist** at the Theoretische Physik, **Universität Paderborn (Germany)** within the DIODE (Designing Inorganic/Organic Devices) RTN in the group of Prof. T. Frauenheim.
- *Sep. 2000-Aug. 2001:* **Visiting scientist** at the Lehrstühl für Theoretische Chemie, **Technische Universität München (Germany)** in the group of Dr. A. Görling.
- *Jan. -Nov. 2002:* Research contract at University of Lecce (Italy).
- *Dec. 2002-Nov. 2004:* tenure-track INFM Researcher at National Nanotechnology Laboratories (NNL), Lecce, Italy.
- *Dec. 2004-Dec. 2009:* **permanent CNR-INFM Researcher** at NNL.
- *Jul.-Oct 2010:* **Visiting Professorship** at **IRIS-Adlershof, Humboldt Universität, Berlin.**
- *Jan. 2010-Jun. 2016: Senior Researcher (Primo Ricercatore) at CNR-NANO-Lecce.*
- *Jun. 2016-Nov. 2016: Research Director (Dirigente di Ricerca) at CNR-NANO-Lecce.*

RESEARCH ACTIVITIES:

Dr. F. Della Sala (FDS) is an expert of theoretical and computational methods for material science. His main research activity is focused on the development and application of **Density-Functional Theory (DFT)** and **multiscale methods** to model electronic, optical and photophysical properties of nanostructures (organic molecules, semiconductor and metal nanoparticles, hybrid interfaces). FDS is also an expert of high performace computing (HPC), both at the hardware and software level. He is a developer of the quantum-chemistry program package TURBOMOLE (www.turbomole.com) since 2002.

FDS is mostly known at international-level for the modelling of **GaN heterostructures**, for the development of GGA, meta-GGA and effective **exact-exchange methods of the DFT,** for the development of **frozen-density embedding** (FDE) methods, and more recently for the development of **kinetic-energy functionals** for orbtial-free DFT. FDS's work on GaN heterostructures have been cited by the 2014 Nobel Prize S. Nakamura, for the invention of efficient blue light-emitting diodes which has enabled bright and energy-saving white light sources.

FDS has been leading, since 2003, the theoretical and computational group of CNR in Lecce (first CNR-INFM, then CNR-NANO, now CNR-IMM) and, since 2009, the Platform Computation of the Center of Biomolecular Nanotechnology (CBN) of the Istituto Italiano di Tecnologia (IIT), with an average group-size of 6-8 people.

In 2007, FDS received the **ERC-Starting Grant,** for the project DEDOM (Development of Density Functional Theory methods for Organic Metal interaction).

CITATION METRICS: (from Google Scholar)

- **200 publications** on international journals (33 publications with Impact Factor>7).
- **>10,000 citations.**
- **h-index=50.**

MAIN RESEARCH PROJECTS:

- **SANANO (Self-Assembly of Shape Controlled Colloidal Nanocrystals),** Feb. 2005–Jan. 2008, coordinated by L. Manna (NNL-INFM-CNR); *Co-investigator in a task-project.*
- **SPIDME (Spintronic Devices for Molecular Electronics),** Nov. 2006–Oct. 2009, coordinated by G. Maruccio (NNL-INFM-CNR); *Co-investigator in a task-project.*
- **DEDOM** (Development of Density functional theory methods for Organic Metal Interaction) **FP7-Ideas, ERC-Starting Grant**, July 2008-Dec. 2013; Principal Investigator.
- **Integrated Multiscale Computational Technology,** Computational Platform of the Italian Institute of Technology (Sept. 2009-Sept. 2014); *Coordinator at CBN.*

SUPERVISION OF STUDENTS AND POSTDOCTORAL FELLOWS:

- **Tutor of 3 Diploma theses** at University of Salento (Physics).
- **Tutor of 9 Ph.D. theses** at University of Salento (Nanoscience).
- **Tutor of 9 postdoctoral fellows** (CNR, IIT).

TEACHING ACTIVITIES:

- University of Salento, Physics Dept.: “Physics of Materials” (teaching assistant), years 2005-2007.
- University of Salento, Physics Dept.: “Solid-State Physics” (teaching assistant), year 2009.
- University of Salento, ISUFI: “Numerical Analysis I” (holder of the course), years 2013-2016.
- University of Salento, ISUFI: “Numerical Analysis II” (holder of the course), years 2013-2016.
- University of Salento, ISUFI: “Numerical Analysis” (holder of the course), year 2017.

EDITORIAL SERVICES:

- **Book Editing:** F. Della Sala and S. D’Agostino, *Handbook of Molecular Plasmonics*, Pan Stanford Publishing 2013, ISBN: 9789814303200, 498 pages.
- Since 2016: **Member of the Editorial Board** of the open-access journal "Computation" (MDPI).

INSTITUTIONAL RESPONSIBILITIES:

- 2003-2018, Responsible of the CNR-NANO-Lecce computing centre.
- Since 2014, **Member of the Ph.D. Committee**, University of Salento, “Physics and Nanoscience”.
- Since 2020, Responsible for the CEMAS (Center for Materials and Atmospheric Simulations).

REFEREE ACTIVITY:

- For Journals: Phys. Rev. Lett., Phys. Rev. B, J. Chem. Phys., Appl. Phys. Lett., J. Phys. Cond. Matt., New. J. Phys., J. Am. Chem. Soc., Chem. Phys. Chem., J. Phys. Chem. C, Int. J. Quantum. Chem., Chem. Phys., J. Phys. Cond. Matter., Sci. Adv. Mater., Nanotechonolgy.
- For grants: National Science Foundation (NSF), Swiss National Science Foundation (SNSF), FWF (Fonds zur Förderung der wissenschaftlichen Forschung, Austria), Romanian National Research Council (CNCS), Italian Institute of Tecnology (IIT) seed Projects.

DEVELOPMENT OF ELECTRONIC STRUCTURE CODES:

- Since 2002, Contributor to **TURBOMOLE** (www.turbomole.com), commercial code.
- Since 2010, Contributor to **ADDA** (http://code.google.com/p/a-dda/), open-source.
- Since 2010, Contributor to **FHI-AIMS** (https://aimsclub.fhi-berlin.mpg.de/), licensed.
- Since 2019, Contributor to **PROFESS** (https://github.com/EACcodes/PROFESS), open source.

COMMISSION OF TRUST:

- Member of the Ph.D. Committee “Fisica&Nanoscienze”, 35th cycle, Unisalento.
- Member of the Ph.D. Committee “Fisica&Nanoscienze”, 32th cycle, Unisalento.

- Member of the Ph.D. Committee "Fisica&Nanoscienze", 29th cycle, Unisalento.
- Opponent for Ph.D. Thesis of Jouko Lehtomäki, Aalto University "*Density functional theory approximations from semiclassical considerations"*. 24-1-2020.

MAJOR INTERNATIONAL COLLABORATIONS (last 10 years):

Prof. P. Gori-Giorgi (Amsterdam), Prof. P. Cortona (Paris), Prof. I Grabowski and Prof. S. Śmiga (Nicolaus Copernicus University, Torun, Poland), Prof. A. Görling (University of Erlangen-Nürnberg), Prof. M. Sierka (Friedrich-Schiller-Universität, Jena), Prof. T. Niehaus (Lyon), Dr. M. Yurkin (Novosibirsk, Russia), Prof. F. Henneberger (Humboldt University, Berlin), Prof. O.L.A. Monti (University of Arizona).

SELECTED INVITED TALK: at national/international conferences/workshops **(5 out of 17)**

- F. Della Sala, "*Electrostatic Field Driven Alignment of organic oligomer of ZnO surfaces"*, **Deutsche Physikalische Gesellschaft (DPG11)**, 13-18/3/2011, Dresden (Germany).
- F. Della Sala ***[key-note]*** *"Non-empirical exchange-correlation functionals with improved accuracy"* **XXV Congresso della societa' di Chimica Italiana (SCI2014),** Rende, 7-11/9/2014.
- F.Della Sala, "*Kohn-Sham kinetic energy density in the nuclear and asymptotic regions"*, The 16th International Conference on Density-Functional Theory and its Applications (**DFT15),** 31/8-4/9/2015, Debrecen (Hungary)
- F. Della Sala, "*Semilocal Kinetic Energy Functionals for Orbital-Free Density Functional Theory"* The 18th International Conference on Density-Functional Theory and its Applications (**DFT19)**, Alicante 22-26/7/2019
- F. Della Sala, "*Ab initio Plasmonics of Externally Doped Silicon Nanocrystals"*, **FISMAT 2019** - Italian National Conference on Condensed Matter Physics , Catania, 30/9-4/10/2019

BOOK CHAPTERS:

- F. Della Sala, *Orbital-Dependent Exact-Exchange Methods in Density Functional Theory*, SPR-Chemical Modelling, Applications and Theory, Volume 7, RSC Publishing, pp.115-161 (2010).
- F. Della Sala, *Foundations of Molecular Plasmonics*, in *Handbook of Molecular Plasmonics*, Pan Stanford Publishing, pp 1-70 (2013).

PATENTS:

M. Ben Khalifa, F. Della Sala, B. Dussert-Vidalet, G. Gigli, V. Maiorano, F. Mariano, M. Mazzeo, *Organic Light Emitting Diode with Microcavity including doped organic layers and fabrication process thereof*, US 8969853 B2

SELECTED PUBLICATIONS (20 out of 200):

(The complete and updated list of publications, citations and metrics can be found on Google Scholar, see http://scholar.google.it/citations?&user=KR6o20AAAAAJ.)

- F. Della Sala, M. Pezzolla, S. D'Agostino, E. Fabiano, *Ab Initio Plasmonics of Externally Doped Silicon Nanocrystals*, **ACS Photonics** 6, 1474-1484 (2019)
- L. A. Constantin, E. Fabiano, F. Della Sala, *Semilocal Pauli–Gaussian Kinetic Functionals for Orbital-Free Density Functional Theory Calculations of Solids*, **J. Phys. Chem. Lett**. 9, 4385 (2018)
- (invited review) F. Della Sala, E. Fabiano, L. A. Constantin, *Kinetic-energy-density dependent semilocal exchange-correlation functionals*, **Int. J. Quant. Chem.** 116, 1641 (2016)
- C. Ciraci, F. Della Sala, *Quantum hydrodynamic theory for plasmonics: Impact of the electron density tail*, **Phys. Rev. B** 93, 205405 (2016)
- F. Della Sala, E. Fabiano, L. A. Constantin, *Kohn-Sham kinetic energy density in the nuclear and asymptotic regions: Deviations from the von Weizsäcker behavior and applications to density functionals*, **Phys. Rev. B** 91, 035126 (2015).

- S. Laricchia, 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. Theor. Comput.** 10, 164 (2014)
- Y. Xie, L. Carbone, C. Nobile, V. Grillo, S. D'Agostino, F. Della Sala, C. Giannini, D. Altamura, C. Oelsner, C. Kryschi, P.D.Cozzoli, *Metallic-like Stoichiometric Copper Sulfide Nanocrystals: Phase- and Shape-Selective Synthesis, Near-Infrared Surface Plasmon Resonance Properties, and Their Modeling,* **ACS Nano** 7, 7352 (2013)
- L. Chiodo, L.A. Constantin, E. Fabiano, F Della Sala, *Nonuniform scaling applied to surface energies of transition metals,* **Phys. Rev. Lett.** 108 , 126402 (2012)
- F. Della Sala, S. Blumstengel, F. Henneberger, *Electrostatic-field-driven alignment of organic oligomers on ZnO surfaces,* **Phys Rev Lett** 107, 146401 (2011)
- L.A. Constantin, E. Fabiano, S. Laricchia, F. Della Sala, *Semiclassical neutral atom as a reference system in density functional theory*, **Phys. Rev. Lett.** 106 (2011) 186406
- S. Laricchia, E. Fabiano, L.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, 2439 (2011)
- N. Baadji, M. Piacenza, T. Tugsuz , F. Della Sala, G. Maruccio, S. Sanvito, *Electrostatic spin crossover effect in polar magnetic molecules,* **Nature Materials,** 8, 813 (2009)
- D. Steiner, D. Dorfs, O. Millo, U. Banin, F. Della Sala, L. Manna, *Determination of Band Offsets in Heterostructured Colloidal Nanorods Using Scanning Tunneling Spectroscopy,* **Nanoletters** 8, 2954 (2008)
- L. Carbone, C. Nobile, M. De Giorgi, F. Della Sala, G. Morello, P.P. Pompa, M. Hytch, E. Snoeck, A. Fiore, I. R. Franchini, M. Nadasan, A. F. Silvestre, L. Chiodo , S. Kudera, R. Cingolani , R. Krahne, L. Manna, *Synthesis and Micrometer-Scale Assembly of Colloidal CdSe/CdS Nanorods Prepared by a Seeded Growth Approach,* **Nanoletters** 7, 2942 (2007)
- P.P. Pompa, L. Martiradonna, A. Della Torre, F. Della Sala, L. Manna, M. De Vittorio, F. Calabi, R. Cingolani, R. Rinaldi, *Metal-enhanced fluorescence of colloidal nanocrystals with nanoscale,* **Nature Nanotech.** 1, 126 (2006)
- M. Mazzeo, V. Vitale , F. Della Sala, M. Anni, G. Barbarella, L. Favaretto, G. Sotgiu, R. Cingolani and G. Gigli, *Bright White Organic Light-Emitting Devices from a Single Active Molecular Material,* **Adv. Mater.** 17, 34 (2005)
- F. Della Sala and A. Görling, *Asymptotic behavior of the Kohn-Sham exchange potential,* **Phys. Rev. Lett.** 89, 033003 (2002)
- F. Della Sala and A. Görling, *Efficient localized Hartree-Fock methods as effective exact-exchange Kohn-Sham methods for molecules,* **J. Chem. Phys.** 15, 5718 (2001)
- T. Niehaus, S. Suhai, F. Della Sala, P. Lugli, M. Elstner, G. Seifert, Th. Frauenheim, *Tight-binding approach to Time Dependent Density Functional Response Theory,* **Phys. Rev. B** 63, 085108 (2001)
- F. Della Sala, A. Di Carlo, P. Lugli, F. Bernardini, V. Fiorentini, R.Scholz, J.-M. Jancu, *Free-charge screening of polarization fields in wurtzite GaN/InGaN laser structures,* **Appl. Phys. Lett.** 74, 2002 (1999)

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