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LILIA BOERI
Curriculum Vitae

Versione priva dei dati sensibili, ai fini della pubblicazione, secondo l’art. 4 del Codice in materia di protezione dei dati personali e dall’art. 26 del D. Lgs. 14 marzo 2013, n. 33.

Rome, 4/8/2024

Part I – General Information

- **Full Name:** Lilia Boeri
- **Google scholar:** https://scholar.google.it/citations?user=DwmLnv4AAAAJ&hl=it
- **Researcher ID**: B-6162-2015
- **Spoken Languages:** Italian (Mother Tongue), English (Fluent), German (Fluent), French (Good)

- **Current Position:** Associate Professor, sector 02/B2 (Theoretical Condensed Matter Physics), Physics Department, Sapienza Universita’ di Roma, Italia (since 27/3/2020).
- **Habilitation** as Full and Associate Professor for sectors **02/B2 (Theoretical Condensed Matter Physics) and 03/A2 (Theoretical Chemistry) - April 2017.**

Part II – Education

Type	Year	Institution	Notes
University graduation	2001	Universita’ la Sapienza, Roma	Diploma di laurea in fisica (VO); 110/110 lode; Thesis: "*Electronic Correlation and Non-Adiabatic Superconductivity*", Supervisor: Prof. L. Pietronero.
PhD	2005	Universita’ la Sapienza, Roma	Dottorato di Ricerca in Fisica, XVII Ciclo; Thesis: “Electron-phonon Interaction in the new s-p Superconductors: Magnesium Diboride and Hole-Doped Diamond", Supervisors: Prof. G. B. Bachelet, Prof. L. Pietronero

Part III – Appointments

IIIA – Academic Appointments

Start	End	Institution	Position
2/2001	9/2001	Universita’ la Sapienza, Roma, Italy	Borsa di studio post-laurea
10/2001	9/2004	Universita’ la Sapienza, Roma, Italy	Borsa di studio per dottorato di ricerca in fisica
2004	2006	Max Planck Institute for Solid State Research, Stuttgart, Germany	Postdoc scholarship (Andersen Department)
2006	2009	Max Planck Institute for Solid State Research, Stuttgart, Germany	Member of the Scientifc Staff (Andersen Department); non-permanent researcher.
2009	2013	Max Planck Institute for Solid State	Head of the Minerva Research Group

		Research, Stuttgart, Germany	"*Computational Approaches to Superconductivity*"; Non-permanent W2 (Associate professor) position; in 2012 my group successfully passed the internal evaluation from the MPI International Scientific Advisory Committee.
2013	3/2017	Institute for Theoretical and Computational Physics, Graz University of Technology, Austria	Tenure-Track Associate Professorship.
3/2017	3/2020	Physics Department, Sapienza Universita' di Roma, Italy	Tenure-Track Associate Professorship (RTDb), Theoretical Condensed Matter (02/B2)
3/2020	today	Physics Department, Sapienza Universita' di Roma, Italy	Associate Professorship (RTDb), Theoretical Condensed Matter (02/B2)

IIIB – Other Appointments

Start	End	Institution	Position
10/2003	7/2004	Max Planck Institute for Solid State Research, Stuttgart, Germany	Visiting PhD student
7/2009	8/2009	Kavli Institute for Theoretical Physics, Santa Barbara, USA	Visiting Researcher
8/2010	8/2010	Riken Japan	Visiting Researcher
1/2011	1/2011	Kavli Institute for Theoretical Physics, Santa Barbara, USA	Visiting Researcher
9/2014	9/2014	Kavli Institute for Theoretical Physics, Santa Barbara, USA	Visiting Researcher
5/2017	10/17	Politecnico di Torino, Italy	Visiting Professor at the Department for Science and Advanced Technologies, Politecnico di Torino, **(**tot. Grant ca. 45 keuro**)** *-turned down as I moved to Rome*

IIIC – Academic Job Offers:

2009	Junior Professorship in Computational Physics (Rechnergestutze Physik) from the Augsburg University, Germany, *turned down*.
2009	Junior Professorship in Theoretical Nanoelectronics from RWTH Aachen, Germany, *turned down.*
2011	Associate Professorship in Theoretical Physics, University Wurzburg, *listed second on the final shortlist.*
2015	Short-listed for a Full Professorship in Theoretical Physics, Heidelberg, Germany.
2022	Short-listed for a Full Professorship in Theoretical Physics, Wuerzburg, Germany.

Part IV – Teaching experience

IVa – University Lectures:

Year	Institution	Lecture/Course
2003/2004	Universita' La Sapienza, Roma, Italy	**Laboratorio di Calcolo (prof. G. Organtini),** teaching Assistant.
2011-12(WS)	University of Stuttgart, Germany	**Electronic Structure Theory 9th semester**, MSC and Phd Students in Physics (7 students) 3 ECTS
2013-2017	Graz University of Technology, Graz, Austria	**Numerical Methods in Technical Physics**, 5th semester (BSC Technical Phyics), physics Lecture + Exercise class (≈90 students/year); lecturer + examiner (I was supported by teaching assistants).* 6 ECTS

2013-2017	Graz University of Technology, Graz, Austria	**Solid State Theory**, 7th semester, (MsC Technical Physics) Lecturer + examiner (≈25 students/year);* 3ECTS.
2013-2017	Graz University of Technology, Graz, Austria	**Band Structure Methods**, 9th semester, (MsC and PhD in Technical Physics) (≈10 students/year); lecturer + examiner.* 3 ECTS.
2017	Sapienza Universita' di Roma	**Statistics** exercises for the course *Physics for chemistry*, bachelor in chemistry, lectures prof. Castellani and Loreto, Sapienza (**AA 2016-17**), 3 ECTS (≈250 students/year)
2017-2024	Sapienza Universita' di Roma	**Laboratorio di calcolo** (lectures and exercises), 6 CFU/ECTS, bachelor in Physics, Sapienza (≈130 students/year)
2019-20	Sapienza Universita' di Roma	**Computing Methods for Physics,** co-lecturer, (G. B. Bachelet, S. Moroni), 6CFU, Master in Physics. (≈30 students/year)
2021-2023	Sapienza Universita' di Roma	**Condensed Matter II,** 6 CFU/ECTS, Master in Physics Sapienza (≈40 students/year)
2023-today	Sapienza Universita' di Roma	**Computing Methods for Physics (now Computational Solid State Physics),** 6 CFU/ECTS, Master in Physics Sapienza (≈60 students/year)

IVb – Other Teaching Activities:

Year	Institution	Lecture/Course
2004	Chalmers University, Goteborg, Sweden	**Instructor** at the "*MPI-Stuttgart/Swedish Midsummer School on Computational superconductivity*", June 23rd-26th 2004.
2006	Duke University (USA)	**Instructor** for a seven-lectures workshop on "Theory and Calculation of Superconducting Materials", sponsored by the Pratt School of Engineering.
2007	Naval Research Lab, Washington DC, USA	**Instructor** for a seven-lectures workshop on "Theory and Calculation of Superconducting Materials",
2009	Chiavari, Italy	**Lecturer** at a INFM National School on "Physics of Spin in Materials", Chiavari, Italy, 2-9 November 2009.
2012	Politecnico di Torino, Italy	**Lecturer** for a course on "ab-initio calculations for superconductors", Politecnico di Torino, Italy, April 2012.
2015	Sissa, Trieste, Italy	**Lecturer** for the master in "comunicazione della scienza".

Part V - Society memberberships, Awards and Honors

Year	Title
1995	Scholarship to cover all expenses for the Physics studies at La Sapienza, Rome (the scholarship was awarded to the top students of my academic year).
1996	Scholarship to cover all expenses for the Physics studies at La Sapienza, Rome (the scholarship was awarded to the top students of my academic year).
2002	Member of the American Physical Society.
2004-5	Scholarship of the Max Planck Society, Germany.
2007-8	Monetary prize for excellent scientific performance, Max-Planck Society.
2008	Member of the German Physical Society.
2010	Member of the PSIK working group for Superconductivity (ESF).
2012	Member of the Humboldt Society (Germany).
2015	Member of the Review Committee for Physical Review B.

2024	Member of the PSIK Board of Trustees (PSIK is an International Organization for the promotion of Electronic Structure Methods worldwide).

Part VI – Student/Postdoc (Co-)Supervision:

Since 2010, I have officially supervised or co-supervised **15 bachelor, 16 master and 7 PhD theses**, and several **postdocs** and research assistants. Some of my previous students and postdocs now hold permanent or tenure-track positions at research and academic institutions worldwide.

VIa: Bachelor, Master and PhD Theses:

2013	PhD Thesis (University of Stuttgart)	Luciano Ortenzi "*Phenomenological approach to spin fluctuations in itinerant magnets and superconductors from ab initio calculations*" – co-supervision, with O.K. Andersen;
2015	Bachelor Thesis	Lukas Hoermann "*Electronic Structure of CaCuO2 in the LSDA+U approximatio*n", 25/11/2015
2015	Bachelor Thesis	Patrick Schiffmann, "*Superconductivity in FCC Aluminum with Density Functional Perturbation Theory using quantum espresso*"(14/7/2015)
2015	Bachelor Thesis	Andreas Theiler, "*Description of the Evolutionary Algorithm for Crystal Structure Prediction and Applications to new phases of borides*" (12/5/2015)
2015	PhD Thesis (Graz University of Technology)	Christoph Heil "*Electronic Properties and Susceptibility Functions of Iron-based superconductors"* – co-supervision, with W. von der Linden. **Now tenure-track associate professor @TU Graz.**
2016	Master Thesis (co-supervision)	Michael Rumetshofer "*First principles molecular transport calculation*", (with W. von der Linden), (25/2/2016).
2016	Bachelor Thesis (TU Graz)	Matthias Gruber, "*Ab initio High-Pressure Phase Diagram of Hydrogen Sulfide*" (19/2/2016)
2016	Master Thesis (TU Graz)	Christian Kokail, "*Superconducting Properties of high pressure lithium-sulfur compounds predicted by evolutionary algorithms*". (now PhD student at the Institute for Quantum Optics and Quantum Information, Innsbruck)
2017	Bachelor Thesis (Sapienza)	Lorenzo Rossi, "*Ab-initio calculations of metal-insulator transition in sodium at high pressures*"
2017	Bachelor Thesis (Sapienza)	Francesco G. Rinaldi, "*Algoritmi evolutivi per lo studio di strutture cristalline*".
2018	Bachelor Thesis (Sapienza)	Valentina Carpenella, "*Studio della transizione isolante-metallo nell'idrogeno solido con metodi ab-initio*".
2018	Master Thesis (Sapienza)	Francesco Lucantoni: "*Study of anharmonicity and zero-point effects in magnesium diboride within the Stochastic Self-Consistent Harmonic Approximation*", (with F. Mauri).
2018	Master Thesis (Sapienza)	Simone di Cataldo *"High-pressure spectroscopy of the hybrid perovskite Formamidinium lead iodide"* (with P. Postorino).
2019	Master Thesis (Sapienza)	Leonardo Ratini, *Study of superconductivity in chromium hydride using Density Functional Theory*" (with P. Postorino).

2019	Bachelor Thesis (Sapienza)	Alessio Cucciari, "*Studio ab-initio di un nuovo composto di elio e sodio ad alte pressioni*"
2019	Bachelor Thesis (Sapienza)	Matteo Peperoni, "*Ricerca di Materiali Superconduttivi con Metodi di Machine Learning*", (with L. Pietronero).
2019	Bachelor Thesis (Sapienza)	Federico Trezzini, "*Studio delle proprietà elettroniche del grafene mediante un modello Tight Binding*"
2019	Bachelor Thesis (Sapienza)	Giovanni Tomasucci, "*Studio delle strutture cristalline dell'idrogeno atomico ad alta pressione con metodi ab-initio*"
2019	Master Thesis (TU Graz)	Franz Martin Rohrhofer, "*Machine Learning of first-principles energies for carbon and boron crystal structures*" (with W. von der Linden).
2019	PhD Thesis (TU Graz)	Andriy Smolyanyuk, "*Electronic Structure of Oxide Heterostructures"* – now Postdoc TU Wien.
2020	Bachelor Thesis (Sapienza)	Danilo de Pauli, "Simulazione dell'evoluzione di un incendio: un'applicazione che utilizza automi cellulari"
2022	PhD Thesis (joint thesis Rome + TU Graz)	Simone di Cataldo, *"Ab-initio materials design of superhydrides: a quest to high-Tc superconductivity at room pressure*", **now Assistant Professor (RTDA @Sapienza).**
2022	Master Thesis (Sapienza)	Alessio Cucciari *"Ab-initio study of high-temperature superconductivity in new ternary sodalite-like clathrate hydrides at high pressures*", Physics, Sapienza, June 2022, now PhD student@Sapienza.
2022	Master Thesis (Sapienza)	Federico Giannessi "*Predizione di nuovi idruri ternari con metodi high-throughput*, Physics, Sapienza, March 2022, now PhD student @ l'Aquila.
2022	Master Thesis (Sapienza)	Paolo Ingelido, "Computation of Kinetic Stability" (January 2023).
2022	Bachelor Thesis (Sapienza)	Francesco Gargiulo, *"Superconduttivita' negli idruri ad alta pressione",* July 2022.
2022	PhD Thesis (Sapienza)	Alessio Cucciari (ongoing)
2022	PhD Thesis (Sapienza)	Flavio Giuliani (ongoing)
2023	Master Thesis (Sapienza + Heidelberg)	Caja Annweiler, "High-Throughput Prediction of Ternary Phase Diagrams: Method Development and First Applications to Ternary Hydrides", October 2023 (with M.W. Haverkort).
2023	Master Thesis (Sapienza + TU Graz)	Eva Kogler, "*Determining the Stability of Topical Superconductors: A Machine Learning-Driven Ab-Initio Approach*", November 2023 (with C. Heil).
2024	Master Thesis (Sapienza)	Dionisia Naddeo, "*Unveiling Anharmonic Phonon Behavior in the NbTi Superconductor from First Principles*", March 2024.
2024	Master Thesis (Sapienza)	Efisio Madeddu, *"Proximity effect in germanene-superconductor",* ongoing.
2024	Master Thesis (Sapienza)	Valerio Tammurello, "*Coexistence of Charge Density Wave and Superconductivity in Rare-Earths Ni-C compounds*", ongoing.
2024	Master Thesis (Sapienza)	Alessio Serafini, "*Template-based method for approximate binary convex hull construction*", ongoing.
2024	Master Thesis (Sapienza)	William Cursio, "*Assessing the accuracy anisotropic Migdal-Eliashberg Theory in Transition Metal Carbides*", ongoing.
2024	Bachelor Thesis (Sapienza)	Matteo Cheri, "*Modello BCS a due gap per la*

		superconduttività degli idruri ad alta pressione", ongoing.

VIb. Supervision of Postdocs:

2010	Juliang Mao, MPI-FKF, Stuttgart, Germany (now Professor @Xiangtan University, China)
2012	Tobias Schickling, MPI-FKF, Stuttgart, Germany
2010-12	Alaska Subedi, MPI-FKF, Stuttgart, Germany **(now permanent researcher CNRS, France).**
3-12/2015	Christoph Heil, TU Graz, Austria (Now Tenure-Track Associate Professor @TU Graz, Austria).
2018-21	Santanu Saha, TU Graz, Austria, 2018-2021 (now Permanent Reseracher at CNRS, France).
2019-20	Cesare Tresca, Sapienza, Italy (**now permanent Researcher at CNR, Italy**).
2019-21	Jose Flores Livas, RTDA, Sapienza (2019-2021) (moved to an industry position).
2023-	Simone di Cataldo, RTDA, Sapienza

VIc. External Referee of PhD Theses:

2012	Audrey Grockowiak, Grenoble, France (advisors: Etienne Bustarret, Thierry Klein)
2014	Andreas Linscheid, Halle, Germany (advisors: Prof. E.K. U. Gross, Dr. A. Sanna)
2015	Arkady Davidov, Halle, Germany (advisors: Prof. E.K. U. Gross, Dr. A. Sanna)
2018	Giorgio de Tomassis, Università degli Studi dell'Aquila (G. Profeta)
2021	Davide Romanin, Politecnico di Torino (G. Gonnelli)
2022	Francesco Belli, University of the Basque Country (Ion Errea)
2024	Trinidad Novoa, Sorbonne, Paris, France (J. Contreras)

Regular member of Bachelor and Master Thesis committees at Graz University of Technology (2013-17) and Sapienza Università di Roma (2017-today).

Part VII - Funding Information [grants as PI or co-PI]

Since 2009, I have obtained over 3 Million euros funding to support my research from different national and international funding bodies.

Research Grants:

Year	Title	Program	Grant value
2009	"Computational Approaches to Superconductivity", **PI** Succesfully passed the mid-term external evaluation from Scientific Advisory Board (2012).	Minerva Program of the Max-Planck Society	1 Million Euro*
2010	"Magnetoelastic Properties of Fe-based superconductors", **PI**	Special Program "Iron Pnictides and Chalchogenides", SPP 1458, German Research Fund, DFG	120 Keuro **
2013	Magnetism and Nematic Phases of Fe-based. Superconductors from DFT+Gutzwiller	Special Program "Iron Pnictides and Chalchogenides", SPP 1458, German Research Fund, DFG	120 Keuro **

	calculations", **co-PI** (PI: Prof. Florian Gebhard, Marburg, Germany)		
2014	*"Collective Phenomena in Oxide Films and Heterostructures";* **PI**; National Collaboration Partners are C. Franchini (Uni Wien) and Alessandro Toschi (TU Wien).	Special Program SFB-VICOM "Vienna", Austrian Science Fund, FWF	422 Keuro ***
2015	*"Search for Superconductivity and Magnetism in MXene Phases", with prof. T. Saha-Dasgupta* (Austrian **PI**)	Funding for an Indo-Austrian cooperation (OEAD-DIST); (Travel and Exchange Grant).	10 Keuro
2017	*"Superhydra", new high-pressure hydrides for Hydrogen Storage and Superconductivity,* **PI**;****	Stand-alone Project, Austrian Science Fund, FWF	523 keuro
2017	*"High-Tc Superconductivity at Extreme Pressures in Ternary Hydrides",* **PI** *(co-PIs: G.B. Bachelet, L. Pietronero, P.Postorino).*	Progetti Medi di Ateneo, Sapienza	35 keuro
2017	*Grant FFABR (Fondo di avviamento alla ricerca per ricercatori),* **PI** *(score 100/100)*	MIUR	3 keuro
2017	*Visiting Professorship,* **PI,** to host Dr. Igor I. Mazin, NRL Washington, USA	Programma Professori Visitatori, Sapienza	5 keuro
2018	*New High-Pressure Phases of Complex Hydrides: High-Temperature Anharmonic Superconductors (**PI**; co-PIs G.B. Bachelet, F. Mauri)*	Progetti Medi di Ateneo, Sapienza	12 keuro
2019	*"SuperIces: New structures and exotic properties of ion doped and gas filled ices",* **co-PI** (PI L.E. Bove; co-PIs: G.B. Bachelet).	Progetti Medi di Ateneo, Sapienza	38 keuro
2020	*"High pressure nano confinement of molecular systems in zeolites: from structural ordering to new functional materials",* **co-PI** (PI: L.E. Bove, co-PIS: G.B. Bachelet, J.A. Flores-Livas)	Progetti Medi di Ateneo, Sapienza	13 keuro
2020	*Assegno di Ricerca, "Towards ambient pressure, high-Tc superconductivity in complex hydrides", Simone di Cataldo* **(responsabile scientifica)**	Bando Assegni di Ricerca di Dipartimento, Ricerca Cat. A, DD. 151/2020	23.6 keuro
2021	*Material Design with High-Performance-Computing: a common startup infrastructure for the condensed matter theory sector*", **PI** (This grant currently provides the basic infrastructure for the	Bando di Ateneo Medie Attrezzature, Sapienza	62 keuro

	Theoretical Condensed Matter Sector of the Physics Department of Sapienza).		
2021	*Atomistic study of the potential energy surface and the configurational entropy of phase-change materials* (co-PI, PI R. Mazzarello)	Progetti Medi di Ateneo, Sapienza	38.5 keuros
2022	*Simulation of the Solid-Liquid and Liquid-Liquid phase transitions in the High-Pressure Phase Diagram of Sulfur with Ab-initio Machine Learning Potentials,* **PI** (Co-PIs: John Russo, Riccardo Mazzarello)	Progetti Medi di Ateneo, Sapienza	11 keuros
2022	Member of the Spoke 6 (PI Riccardo Mazzarello)	CN1-MIUR-PNRR	Around 40 keuros
2022	Sapienza Leader of Spoke 9, Advanced Material Modelling, and National Coordinator of activities on Superconductivity and Magnetism	PE2-MIUR PNRR	722 Keuros
2022	ERC Synergy Grant HighBOOST, **PI**, co-PIs Mikhail Eremets, Paul Canfield, **Total Budget: 12.529.000 euros**	European Research Council (EU-Synergy call 2023)	Not funded due to insufficient budget (ranked A)
2023	ERC Synergy Grant Decompress, **PI**, co-PIs Mikhail Eremets, Paul Canfield, **Total Budget: 13.628.000 euros**	European Research Council (EU-Synergy call 2024)	Not funded (ranked B)
2023	*"Multi-scale theoretical analysis of realistic Germanium-superconductor interfaces",* co-PI, PI Bernhard van Heck	Progetti Medi di Ateneo, Sapienza	12 keuros

* Funding for own position (W2 German scheme), 2 PhD students, 1 Postdoc, Equipment and consumables for 5 years.
** This amount corresponds to one PhD student position for 3 years.
*** 3 PhD students for 3.5 years + miscellaneous expenses
**** The administrative management of the project had to be transferred by my Institute Head, Prof. Wolfgang von der Linden, upon moving to Sapienza, due to the lack of an international agreement between Austrian and Italian funding schemes.

HPC grants (Computing time):

Since 2017, I've obtained several type C grants from CINECA to support my Master students' projects.
In addition, I have obtained the following grants as main/co-investigator:
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2018	Iscra-B Project, HiTS-EPH, 1.000.000 CPU Hours (PI)
2024	EuroHPC-Prace Project "EXChess", 10.000.000 CPU hours; (co-PI, PI Simone di Cataldo).

Part VIII – Research Activities

VIII a: Schematic Summary

Keywords	***Brief Description (citations refer to Google Scholar, August 2024)***
Superconductivity, DFT, MgB2, Small-Fermi energy effects, many-body theory	Investigated the role of small Fermi energy effect in **magnesium diboride** (MgB2): phonon anharmonicity (Phys. Rev. B 2002), zero-point motion (Phys. Rev. B 2005).
Superconductivity, DFT, Tetrahedral Superconductors	First explanation and prediction of superconductivity in **boron-doped tetrahedral semiconductors** *(Phys. Rev. Lett. 2004),* more than 280 citations.
Superconductivity, DFT, Electron-Phonon Interaction, Downfolding, Intercalated Graphites, specific heat, high pressures.	Explained the role of the interlayer band in the superconductivity of **intercalated graphites**; prediction of experimental trends. (Phys. Rev. Lett. 2006 and 2007, Phys. Rev. B 2006 and 2007) >500 total citations).
Superconductivity, DFT, neutron scattering	**Kohn Anomalies** in elemental superconductors (Phys. Rev. Lett. 2006, Science 2008, 110 total citations).
Superconductivity, DFT, electron-phonon interaction; magnetism; spin fluctuations; many-body; strong electronic correlations.	**Iron-based superconductors:** ruled out electron-phonon interaction as a possible mechanism for superconductivity in iron superconductors (Phys. Rev. Lett. 2008, PRBR 2010); wrote a review on the electronic structure and magnetism (Annalen der Physik 2011); first calculation of the effect of magnetism on the ep interaction (Phys. Rev. B 2010); investigated the role of electronic correlations on magnetism (*Phys. Rev. Lett. 2012, Phys. Rev. Lett. 2015*) – *more than 2000 total citations and 25 invited talks since 2008.*
DFT, many-body, methods, magnetism, strongly correlated electron systems.	Contributed to the development and application of **DFT+Gutzwiller** method for magnetic system, first with downfolded Hamiltonians (*Schickling, PRL 2012*), and then with scf calculations (*Schickling, PRB 2015*) (>60 citations).
Evolutionary DFT Crystal Structure Prediction, superconductivity, hydrides, high pressure, li-rich solids.	**High-Tc Superconductivity at High-pressures in binary and ternary hydrides:** Investigated the role of bonding in H3X chalchogenides (Phys. Rev. B Rapid 2015) and sodalite clathrate YHx hydrides (Phys. Rev. B Rapid 2019) First theoretical explanation of high-pressure phases and superconductivity in high-pressure phosphines (*Phys. Rev. B Rapid 2016, Flores*) and Li-S compounds *(Phys. Rev. B Rapid 2016, Kokail)*; First unbiased calculations of ternary phase diagrams of borohydrides with evolutionary crystal structure prediction (Kokail PRM 2017, Di Cataldo PRB 2020) – *400 citations.*
Evolutionary DFT Crystal Structure Prediction, high pressure, magnetism, charge disproportionation, transition metal oxides.	**New structures of Transition Metal Oxides:** Investigated charge disproportionation in bismuth oxides (Smolyanyuk PRB 2017 and 2018); predicted new 2D layered iridate with exotic magnetic properties (Smolyanyuk PRB 2019).
Metadynamics; DFT linear response; high-throughput screening.	**Novel B/C compounds for high-Tc superconductivity and other applications:** Explored the B/C phase diagram, identifying new superconducting and superhard structures; (Saha PRB 2020, PRM 2021, Di Cataldo PRB 2022) – over 100 citations since 2020.
Evolutionary DFT Crystal Structure Prediction, high pressure,superconductivity, high-throughput screening, Transition Paths, kinetic stability	**Towards room-pressure high-Tc Superconductivity in Ternary Hydrides:** Proposed a new family of high-Tc ternary hydrides stable close to room pressure, identified a new method to estimate thermodynamic stability of metastable phases, using variable cell nudged elastic bands calculations (DiCataldo PRBL 2021, NPJ CM 2022, Lucrezi NPJ CM 2021, Lucrezi Comm. Phys. 2022) – > 200

	citations since 2021.
Editorial & Review Activities	Wrote one of the most extensive **reviews** on high-pressure superconductivity, covering both experimental and theoretical aspects (Flores, Phys. Rep. 2020); coordinated the **2021 Room Temperature Superconductivity Roadmap** (Boeri et al., JPCM 2022) *(> 600 citations since 2020*).
Accelerated Crystal Structure Prediction/ High-Throughput screening	Proposed **multitemplate method** to accelerate crystal structure prediction, implemented computer workflow for high-throughput screening and prediction of materials (Saha et al., Phys. Rev. Mat. 2023; Giannessi et al., Scientific Data 2024).
Evolutionary DFT Crystal Structure Prediction, high pressure,superconductivity, high-throughput screening,	**Debunked Dias' claim of Room-Temperature Superconductivity** in Lu-N-H (Ferreira et al., Nat. Comm. 2023).

VIII b: Extended Description:

My main research focus is **Computational Superconductivity**, i.e. the study and design of novel superconductors through **quantum-mechanical electronic structure calculations, many-body methods, and artificial intelligence techniques**. I have contributed significantly to this field, from identifying the first microscopic material trends in carbon- and boron-based materials in the early 2000s to predicting synthesis conditions and superconducting properties of high-Tc hydrides in recent years. Below is a brief chronological overview of my research evolution, with references to my full publication list and citation counts from Google Scholar (August 2024).

Superconductivity, one of the oldest problems in condensed matter physics, has seen impressive progress in the last twenty years, largely driven by computational methods. A key challenge is to identify materials that can superconduct at temperatures high enough for practical applications, with high-Tc superconductivity conventionally defined as above 77 K—far below the 300 K required for room-temperature superconductivity. When I entered the field at the beginning of my PhD in 2000s, high-T_c research was dominated by cuprates, which at the time were the only known superconductors with critical temperatures exceeding 77 K. Cuprates have a complex phase diagram where phenomena such as magnetism and charge density waves coexist with superconductivity, making their microscopic description extremely challenging. Despite extensive research, a quantitative theory of cuprate superconductivity is still missing; moreover, their two-dimensional nature limits their practical applications.

Although I was involved in the study of Fe-based superconductors, which, like the cuprates, are unconventional superconductors, my research has mainly focused on conventional superconductors described by the Migdal-Eliashberg theory of phonon-mediated superconductivity. Since the discovery of superconductivity in magnesium diboride (MgB_2) in 2001 (*J. Nagamatsu et al., Nature **410**, 63, 2001*), more and more advanced computational methods have been developed to bridge the gap between the many-body Eliashberg theory and actual materials, allowing for first-principles calculations of anisotropic electron-phonon and Coulomb interactions. These methods, combined with modern crystal structure prediction techniques, have led to accurate material predictions [71] as evidenced by the enormous acceleration in superconductor discoveries following the report of high-Tc superconductivity in SH3 (*A. P. Drozdov et al., Nature 525, 73, 2015*).

Here is a short list of my main achievements in the field.

Covalent Superconductors: In the early 2000s, a wide-spread belief held that the maximum T_c attainable via the conventional electron-phonon mechanism was around 25 K, known as the Cohen-Anderson limit. This assumption underestimated the range of relevant parameters, such as phonon frequencies and electron-phonon matrix elements, achievable in real materials. The discovery of MgB_2, with a Tc of 39 K, demonstrated that superconductivity in covalent metals could exceed this limit. This was further supported by the discovery of superconductivity in boron-doped diamond (E.*A. Ekimov, Nature 428, 542, 2004*). I formalized these ideas in a paper published at the end of my PhD with Jens Kortus and O.K. Andersen [66] which has now received almost 300 citations since 2004. Using linear response calculations and an analytical model for electron-phonon interaction and anharmonicity that I had developed earlier [68] we linked the mechanisms of superconductivity in diamond and MgB2 and predicted trends in other B-doped superconductors, later confirmed experimentally (*E. Bustarret et al., Nature 444, 465, 2006*). These works had a long-lasting impact on the field and are still cited, because, in the following15 years, superconductivity in covalent metals and anharmonicity have proved to be two key concepts understand superconductivity in high-pressure hydrides.

Intercalated Graphites: The discovery of MgB_2 led to a renewed interest in studying superconductivity in light-element materials. In late 2005, superconductivity was reported in two intercalated graphites (YbC_6 and CaC_6); the Cambridge group highligthed an unexpected correlation with the filling of a free-electron-like band absent in pure graphite (*T.E. Weller et al., Nat. Phys. 1, 39, 2006*), which contradicted the newly-acquired view that strong electronic bonds were necessary for conventional superconductivity. In 2006-2007, we used linear response calculations and the NMTO-downfolding method, to show that interlayer states, when confined by

an intercalant, lose their free-electron nature and experience strong electron-phonon coupling with out-of-plane phonons. This leads to an inverse dependence of Tc on interlayer separation, a result by R.K. Kremer's experimental group [58,59,61,63]This mechanism also explains superconductivity in single-layer graphene, observed later (*B.M. Ludbrook et al., PNAS 112, 11795, 2015*). My work on intercalated graphites has received around 600 total citations since 2006.

Fe-based Superconductors: The discovery of a Tc of 26 K in F-doped LaOFeAs by the Hosono group in 2008 marked a major breakthrough in superconductivity research - *Y. Kamihara et al., JACS 130, 3296, (2008*), initiating the so-called *iron age of superconductivity.* Like cuprates, tje Fe-based superconductors (FeBSC) are layered materials with a complex phase diagram where superconductivity coexists with magnetism. In an early paper following Hosono's report, I demonstrated that the electron-phonon interaction in LaOFeAs was insufficient to explain its superconductivity, implying that another pairing mechanism must be at work [54]. The initial estimate was later refined to include magnetic fluctuations [52]. Both papers were extremely influential at the time, as they steered the research into alternative scenarios based on spin-fluctuations. 15 years after the original publication, they have been cited over 1000 times. A second line of activity, initiated around the same time in collaboration with Igor Mazin and O.K. Andersen, concerns the problematic description of magnetism in these compounds, due to the strong spin fluctuations. [42,47,53]

All in all, my research on Fe-based superconductors obtained a substantial international recognition, as testified by citations and invited talks at conference and workshop. It had also a strong impact on my career, since, in recognition of my pioneering work, I was invited to participate in the Special Program on Fe-based Superconductors of the German Physical Society in 2008 and the Max Planck society awarded me a Minerva Grant to start my independent group on Computational Approaches to Superconductivity in 2009.

High-Pressure Hydrides: The discovery of high-T_c high-pressure superhydrides represented a major turning point in the history of superconductivity, marking the first time in over a century that a major experimental breakthrough was anticipated by theoretical predictions rather than the other way around. In 2015, Eremets' group reported that a mixture of hydrogen sulfide and molecular hydrogen, when pressurized up to 200 GPa in a diamond anvil cell, formed a new hydride (SH_3) with an unprecedented Tc of 203 K (*A. P. Drozdov et al., Nature 525, 73, 2015).* A few months earlier, a theoretical paper provided a highly accurate first-principles prediction of superconductivity in pressurized sulfur-hydrogen, based on a combination of ab-initio methods for superconductivity and crystal structure prediction, techniques that I developed over the past decade - *D. Duan et al., Sci. Rep. 4, 6968, 2014*.
This powerful combination of computational methods which allows to predict both the thermodynamics and the critical temperature of hypothetical superconductors has now transformed the field of superconducting material research, leading to an unprecedented synergy between theory and experiment [71].

My group has played a major role in this field, publishing more than 20 papers in 10 years, with over 1500 citations, including an invited review [71]. Our work generated a substantial international resonance, as testified by several press releases and invited talks at major international conferences worldwide, such as the PSIK general conference 2015, Gordon Research Conference on Superconductivity in 2019 and High Pressure in 2024, the March Meeting of the American Physical Society in 2020 and 21 and 2024, the AIRAPT conference in 2023.
In these works, I leveraged on my extensive expertise in the application of electronic structure methods to the understanding of microscopic material trends in conventional superconductors to guide the search for better materials at high pressure. An important aspect is the use of crystal structure prediction methods (metadynamics and evolutionary algorithms) to predict the occurrence of unusual stoichiometries and bonding environments at high pressures (forbidden chemistry).
The main highlights of this period are: (1) the explanation of superconducting mechanisms in the two main classes of high-pressure binary hydrides, (covalent and sodalite-clathrates);[17,34] (2) highlighting the role of metastable phases in the superconducting phase diagrams of high-pressure superconductors; [26,33] (3) the prediction of a new class of ternary sodalite clathrates, which require an order-of-magnitude lower stabilization pressure than binary clathrate hydrides to attain high-Tc superconductivity. [2,9,11,13] These works also

introduced important conceptual and methological advances which are now considered established in the field, such as enhanced chemical precompression, kinetic stability, and the use of machine-learning potentials to improve the accuracy of anharmonic phonon calculations.

This research has been largely funded by a stand-alone project of the Austrian Science Fund, Superhydra, obtained just before moving to Italy, and subsequently by grants from Ateneo calls and CINECA in Rome. My work has attracted substantial media coverage. Major outlets such as *Nature* and *New Scientist,* but also the general press (*New York Times, il Manifesto*) have featured our contributions, further validating the impact of our findings and their relevance to the broader scientific community.

Mentoring and Collaboration: In addition to my research, I have mentored several master's and PhD students who have gone on to make significant contributions to the field. Some of my former students and postdocs have established their own research groups. I maintain a strong collaboration with Christoph Heil, Santanu Saha, and Cesare Tresca, aws well as with some of my long-term collaborators, like Antonio Sanna (MPI Halle) and Gianni Profeta (L'Aquila).

Current Projects: My current projects focus on the prediction of **practically-usable superconductors.** I am convinced that in the next few years, essential breakthroughs in superconductor discovery will increasingly emerge from a strong interaction between experiment and theory, as well as from novel possibilities opened by high-throughput computational screening [71]. **These ideas were behind my decision to apply for an ERC Synergy Grant with Paul Canfield and Mikhail Eremets, in both 2023 and 2024,** and to successfully participate in a EUROPrace HPC call this year for high-throughput superconductor search. I have also started discussing directly with researchers in applied superconductivity who are interested in understanding largely-used low-Tc superconductors, where a microscopic understanding of superconductivity is still missing [P1]. I was recently invited to present the basic principles of superconductor design at the European Conference for Applied Superconductivity (EUCAS) and at the IOP School of Superconductivity in Oxford, where I had the chance to connect with representatives from the superconductivity industry and startups. This research also aligns with the goals of the PE2 NEST project of the National Resilience and Recovery Plan, aimed at developing materials for the Energy Transition, in which I have participated since 2022. I am also convinced that the increased technological interest in superconductors requires even more rigorous standards for research. This conviction led me to actively engage in debunking the Rochester group's recent claims of room-temperature superconductivity [4], which have been identified as one of the major scientific controversies of recent years.

Vision and Impact: When I started working in this field more than 20 years ago, there was considerable skepticism about the practical value of theoretical predictions in material research. Now, we have reached a point where detailed material predictions can be made with confidence, and verified experimentally. I consider it a major achievement that experimentalists now trust computational predictions to the point of writing common grants, and I find it even more incredible that we are beginning to engage with industry. Although there have been major scandals, I believe this is a golden age for anyone working in this field, as we are now reaping the fruits of two decades of research. My decision to remain in the field for so long has been driven by the continuous progress. The possibility to contribute to a field that has seen such substantial advancements and to be part of its future evolution is both fulfilling and inspiring.

I believe that the Condensed Matter Sector of the Physics Department of Sapienza, with its strong tradition of research in superconductivity, electronic structure methods and statistical mechanics and will be an ideal setting for this type of research.

Part IX– Summary of Scientific Achievements

IXa. Publications:

(full list of publications and presentations are available in section XIII and XIV respectively).

Product type	Number	Data Base	Start	End
Papers [international]	83	Scopus (Google Scholar)	2000	2024
Book chapter	1	Scopus (Google Scholar)	2000	2024

Total Impact factor (IF)	376.3
Total Citations	4140 (5634)
Average Citations per Product	50 (68)
Hirsch (H) index	34 (39)
Normalized H index*	1.8 (2)

*H index divided by the academic seniority.

Editor on two special issues of Journal of Physics Condensed Matter: *"Novel Superconducting and Magnetic Materials"* and "*The 2021 Room-Temperature Superconductivity Roadmap*".

IXb. Presentations:

Product type	Number
Presentations (invited)	87

Of which:

Invited talks at International Conferences	63
Invited Seminars and Kolloquia	35

Recent invited talks include the Annual American Physical Research March Meeting 2020, 2021, 2024, GRC for Superconductivity (2019) and High Pressure (2024). **A full list can be found in Part XIV.**

Part X– Selected Publications

List of publications selected for the evaluation in pdf format (16) – Citations are extracted from Scopus (29/7/2024).

1. P. P. Ferreira, L. J. Conway, A. Cucciari, S. Di Cataldo, F. Giannessi, E. Kogler, L. T. F. Eleno, C. J. Pickard, C. Heil and L. Boeri, *Search for ambient superconductivity in the Lu-N-H system*, Nature Comm. **14**, 5367 (2023) – ***Editor's Suggestion.***
   Journal IF: 9.7 Citations: 32
   Press Release: Michael Banks, *Superconductivity damaged as researchers look to move on from retractions*, Physics World, 2023.
2. R Lucrezi, E Kogler, S Di Cataldo, M Aichhorn, L Boeri, C Heil, *Quantum lattice dynamics and their importance in ternary superhydride clathrates*, Communications Physics **6**, 298 (2023).
   Journal IF: 5.5 Citations: 6
3. S. Saha, S. Di Cataldo, F. Giannessi, A. Cucciari, W. von der Linden, and L. Boeri, *Mapping superconductivity in high-pressure hydrides: The Superhydra project*, Phys. Rev. Materials **7**, 054806 (2022).
   Journal IF: 3.73 Citations: 5

4. C. Tresca, G. Profeta, G. Marini, G.B. Bachelet, A. Sanna, M. Calandra, L. Boeri, *"Why Mercury is a superconductor",* Phys. Rev. B **106**, L180501 (2022) – **APS highlight of the year 2022.**
   Matteo Rini, "Explaining Mercury's Superconductivity 111 years later", APS Physics
   Journal IF: 3.7 Citations: 4
   Press/Media Releases:
   - Matteo Rini, *"Explaining Mercury's Superconductivity 111 years later"*, APS Physics **15**, s155 (2022) (https://physics.aps.org/articles/v15/s155);
   - Isabelle Dumé, "*Mercury's Superconductivity explained at long last"*, PhysicsWorld (2022);
   - Wikipedia, *Mercury, Element.*
5. R. Lucrezi, S. di Cataldo, W. von der Linden, L. Boeri and Christoph Heil, *"In-silico synthesis of lowest-pressure high-Tc Superhydrides",* NPJ Computational Materials, **8**, 119 (2022).
   Journal IF: 9.7 Citations: 32
6. S. di Cataldo, W. Von der Linden, L. Boeri, *"First-principles search of hot superconductivity in La-X-H ternary hydrides",* Nature Partner Journal Computational Materials, **8**, 2 (2022).
   Journal IF: 9.7 Citations: 26
7. S. di Cataldo, S. Qulaghasi, G. B. Bachelet, L. Boeri, *"High-T_c Superconductivity in doped boron-carbon clathrates"*, Phys. Rev. B **105**, 064516 (2022).
   Journal IF: 3.7 Citations: 31
8. S. Di Cataldo, C. Heil, W. von der Linden, and L. Boeri, *"$LaBH_8$: Towards high-Tc low-pressure superconductivity in ternary superhydrides"*, Phys. Rev. B **104**, L020511 (2021) (Letter)
   Journal IF: 3.91 Citations: 105
   Press/Media Releases:
   - Matteo Rini, "*Easing the Squeeze on Superconductors*", APS Physics, **14**, 46 (2021);
   - Emily Conover, "*Can room-temperature superconductors work without extreme pressure?*", Science News (2021);
   - Ethan Siegel *"How close are we to the holy grail of Room-Temperature Superconductors ?"*, Forbes (2021);
   - Wikipedia, *Lanthanum Decahydride*.
9. J. A. Flores-Livas, L. Boeri, A. Sanna, G. Profeta, R. Arita, M. Eremets, "*A perspective on Conventional Superconductors at High Pressures: Methods and Materials*", Physics Reports **856**, 1-78 (2020).
   Journal IF: 25.6 Citations: 310

   Press/Media Releases:
   Spektrum der Wissenschaft,Weltrekord bei 15 Grad, (Robert Gast)
   https://www.spektrum.de/news/weltrekord-bei-15-grad/1782155;
   - Dipartimento di Fisica, Sapienza, press release:
     https://www.phys.uniroma1.it/fisica/archivionotizie/predicting-and-synthesizing-high-temperature-superconductors-high-pressures-review;
   - Wikipedia: https://en.wikipedia.org/wiki/Superconductivity

10. C. Heil, S. di Cataldo, G.B. Bachelet, and L. Boeri, "*Superconductivity in sodalite-like" yttrium hydride clathrates*, Phys. Rev. B **99**, 220502 (R), (2019).
    Journal IF: 3.6 Citations: 93
11. J. A. Flores-Livas, A. Sanna, A. P. Drozdov, L. Boeri, G. Profeta, M. Eremets, and S. Goedecker, *Interplay between structure and superconductivity: Metastable phases of phosphorus under pressure*, Phys. Rev. Materials **1**, 024802 (2017) - ***Editor's suggestion***.
    Journal IF: 2.84 Citations: 51
12. "*A disorder-enhanced quasi-one-dimensional superconductor*", A.P. Petrović, D. Ansermet, D. Chernyshov, M. Hoesch, D. Salloum, P. Gougeon, M. Potel, L. Boeri, C. Panagopoulos, Nature Communications*, **7,*** (2016);
    Journal IF: 12.12 Citations: 54
13. "*Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure*", José A. Flores-Livas, Maximilian Amsler, Christoph Heil, Antonio Sanna, Lilia Boeri, Gianni Profeta,

Chris Wolverton, Stefan Goedecker, and E. K. U. Gross, Phys. Rev. B **93**, 020508(R) (2016). ***(Editor's suggestion)***.
Journal IF: 3.84 Citations: 119

14. *"Reentrant Phase Coherence in Superconducting Nanowire Composites*", Diane Ansermet, Alexander P. Petrović, Shikun He, Dmitri Chernyshov, Moritz Hoesch, Diala Salloum, Patrick Gougeon, Michel Potel, Lilia Boeri, Ole Krogh Andersen, and Christos Panagopoulos, ACS Nano **10**, 515 (2016).
Journal IF: 13.94 Citations: 13
15. "*Influence of bonding on superconductivity in high-pressure hydrides*", Christoph Heil and Lilia Boeri, Phys. Rev. B **92**, 060508(R) (2015).
Journal IF: 3.72 Citations: 92
Press Release:
    - Edwin Cartlidge, *"Superconductivity record sparks wave of follow-up physics",* Nature **524**, 277 (2015).
16. "*Structural origin of the anomalous temperature dependence of the local magnetic moments in the $CaFe_2As_2$ family of materials*", L. Ortenzi, H. Gretarsson, S. Kasahara, T. Shibauchi, K. D. Finkelstein, W. Wu, S.R. Julian, Young-June Kim, I. I. Mazin and L. Boeri, Phys. Rev. Lett. **114**, 047001 (2015).
Journal IF: 7.65 Citations: 28

Part XI – Interviews and Press Releases

O1. Davide Castelvecchi, *Why superconductor research is in a 'golden age' — despite controversy*, Nature, 16/11/2023.

O2. Martin Schlak, *Die Weltsensation, die keine war*, der Spiegel, 16/11/2023.

O3. Alex Wilkins, *Superconductor hopes dashed after journal retracts 'red matter' study*, New Scientist, 8/11/2023.

O4. Michael Banks, *Superconductivity 'damaged' as researchers look to move on from retractions*, Physics World, 20/10/2023.

O5. L. Boeri, Round table on Room Temperature Superconductivity, EUCAS, Bologna (youtube: https://www.youtube.com/live/wV0t76cc6ts?si=Aegyp-Ii8Bd4JX0U).

O6. K. Chang, *New Study Bolsters Room-Temperature Superconductor Claim, New York Times, 24/6/2023.*

O7. Robert Service, *'Revolutionary' blue crystal resurrects hope of room temperature superconductivity*, Science **379** (2023).

O8. Dan Garisto, *Allegations of Scientific Misconduct Mount as Physicist Makes His Biggest Claim Yet*, Physics **16**, 40 (2023).

O9. Andrea Capocci, *Superconduttività, rivoluzione o fake news?*, Il manifesto, 12/3/2023.

O10. *Science, online edition: http://www.sciencemag.org/news/2009/05/new-high-temperature-superconductors-feel-familiar-vibe;*

Part XII– Other Activities (Service)

XII a: Service for International Bodies and Institutions:

- **Scientific Host** for a Humboldt Research Grant awarded to Dr. Igor Mazin from Humboldt society, Stuttgart, 2013.
- **Referee** for the Italian Ministry for University and Research (MIUR), ANVUR NS PRIN project (2012-13).
- **Referee** for the German Physical Society (DFG) and Humboldt Foundation (Germany), National Science Foundation (USA).
- **Member** of the PSIK working group for Superconductivity (2010-17). **Since 2017**: **Leader** of the PSIK working group for Solid State Spectroscopies. PSIK is an international network for the advancement of computational physics (http://psi-k.net/).

- **Since 2024:** Member of the PSIK Board of Trustees.
- European **member of the *Visiting Committee*** of Physical Review B (2016) at the APS Headquarters, Brookhaven, USA.
- **Referee** for Nature Physics, Nature Chemistry, Nature, Physical Review Letters, Physical Review B, Physica C, European Journal of Physics B, Journal of Low Temperature Physics, …
- **Member of the Editorial Board** of Journal of Physics Condensed Matter, Electronic Structure Sector, Institute of Physics, UK.

XII b: Service at my Own Institutions (MPI Stuttgart, TU Graz, Sapienza):

- **Vice-representative** of the scientific staff, Max-Planck Institute for Solid State Research, Stuttgart (2012-13).
- Co-organizer of the **Grazer Physikalisches Kolloquium** (with Markus Aichhorn), 2013-15.
- Member of a Tenure-Track Associate Professor (Laufbahnstelle) Committe, Institute for Solid State Physics, TU Graz (2016).
- Member of the Entrance Committee for the PhD in Physics, XXXIV cycle, with G. Organtini (Chairman) and F. Ricci Tersenghi (**2018**).
- Member of the hiring committee for Sapienza postdoc scholarship (2017): Bando nr 75-design 76/2017 (Santini, Raggi), 135/2018 (Bachelet, Moroni) (2018), (Bachelet, Sciortino).
- Responsible for the design of the Web page of the Physics Department, Sapienza Universita' di Roma, 2017-19 (with Paolo Pani).
- Member of the Editorial board for the Scientific Report of the Physics Department, Sapienza Universita' di Roma, 2016-19 (with L. Baldassarre, I. di Palma, L. La Magna, M. Nardecchia, M. Raggi).
- Member of the Committee for the Evaluation of Teaching Quality, Physics Department, Sapienza (2021-)
- Member of the Organizing Committee of the International Women in Science Day, Sapienza, 2019 and 2021.
- Responsible for the Maintenance of the Computer Lab, Physics Department, Sapienza (with C. de Michele) – 2020 to 2024.
- Founding Member of the **Gender Equality Plan Committee**, Sapienza, 2022-23 – stepped down when elected to the Department Board.
- Member of the **Committee for the Three-Year Strategic Plan** of the Physics Department (2023), Phyiscs Department, Sapienza.
- Member of the **Department & Faculty Board** (Giunta di Facoltà e Dipartimento), Physics Department, Sapienza 2022-.

XII C: Organization of International Conferences and Workshops:

2010: Workshop "Electronic Structure of Fe-based Superconductors", held at the MPI for Solid State Research, Stuttgart. (Local scientific organizer, together with O.K. Andersen, I. Mazin, H. Rosner). Finanziamento totale: 28 keuros Max-Planck-Society (Germany), PSI-K (UK), ONRG (USA).

2011: Workshop "SYLCA 100" (Superconductivity 100 Years Later: a Computational Approach), Alghero (Italia), 15-18 Settembre 2011 (Scientific Organizer, with S. Massidda and E.K.U. Gross). Total funding: 25 keuros from CECAM (EU), PSI-K (UK), ONRG (USA), Regione Sardegna (Italy).

2014: First CECAM-Lorentz workshop "Towards room-temperature superconductivity", Lorentz Center, Leiden, Holland, July 2014; (scientific co-organizers: Hardy Gross, A. Sanna). Total funding: 28 keuros from CECAM (EU), PSI-K (UK), Max-Planck Society (Germany); 25 participants.

2015: Workshop on "*Computer Simulations for Condensed Phase Systems*", Rome, CNR, May 2015. Total Funding: 15 keuros from PSI-K (UK), ERC (EU), CNR (Italy), IBM (Italy). Scientific organizer, together with P. Alippi, C. Attaccalite, F. Affinito, L. Guidoni, D. Varsano.

2017: VICOM winter school on Computational Magnetism, Vienna, Austria *(90 applicants, 60 accepted (registered) participants);* Total Funding: 15 keuro. Austrian Science Fund, Co-organizers: C. Franchini, P. Mohn, A. Toschi.

2017: 652nd Wilhelm-Elsa Heraeus Seminar "*Ab-initio solid state physics in the 21st century*", finanziato da Heraeus foundation (Germania); findanziamento totale 29 keuros. Co-organizers: Igor I. Mazin, T. Saha-Dasgupta, R. Valenti.

2018: "RomeSC2018, International Workshop on Electronic Structure of Superconductors and Novel Materials", 23-25 Maggio 2018, presso Sapienza Universita' di Roma, Italia, financed by Physics Department, Sapienza; Politecnico di Torino, Frankfurt University. Co-organizers: Giovanni B. Bachelet, Renato Gonnelli, Igor Mazin, Roser Valenti.

2020: "*Recent Developments in Quantum Montecarlo Methods*", (with F. Affinito, G.B. Bachelet, D. Ceperley, G. Senatore), financed by Sapienza, PSIK, Cecam. (postponed to **2021**)

2020: "*Challenges in Designing Room Temperature Superconductors*", with R. Hennig, P. Hirschfeld, G. Profeta, A. Sanna, financed by Universita' dell'Aquila, PSIK, CECAM, NSF, postponed to **2022**.

2022: Member of the Scientific Committee for the Annual PSIK conference **2022** (this is the largest European conference on Electronic Structure Methods, held every 5 years).

2022 Member of the M2s-2022 Program Committee Vancouver (this is the largest international conference on Superconductivity).

2025: Member of the Program Committee for the 2025 PSIK conference (this is the largest European conference on Electronic Structure Methods, held every 5 years).

2025: Organizer of a Workshop on "*Challenges in Designing Room Temperature Superconductors*", with R. Hennig, P. Hirschfeld, G. Profeta, A. Sanna, R. Arita, E. Zurek, financed by Sapienza, PSIK, Japanese Science Fund, NSF (USA).

Part XIII – Full List of Publications

Submitted Articles available as preprints:

P1. A. Cucciari, D. Naddeo, S. di Cataldo and L. Boeri, "*NbTi: a nontrivial puzzle for the conventional theory of Superconductivity*", arXiv:2403.15196 (submitted to Phys. Rev. Lett.)
P2. F. M. Rohrhofer, S. Saha, S. di Cataldo, B. C. Geiger, W. von der Linden and L. Boeri, "*Importance of feature engineering and database selection in a machine learning model: a case study on carbon crystal structures*", arxiv:2102.00191 (submitted to Phys. Rev. Mat.)
P3. S. Saha, W. von der Linden and L. Boeri*, Comment on Pentadiamond: "a Hard Carbon Allotrope of a Pentagonal Network of sp2 and sp3 C atoms*", arxiv:2007.09254 (*submitted to Phys. Rev. Lett.; the original paper was retracted after receiving our and two other comments*).

Articles on International Journals (with Referee):

1. F. Giannessi, S. di Cataldo, S. Saha and L. Boeri, "*HEX: High-pressure Elemental Xstals, a complete Database*", NPG Scientific Data **11**, 766 (2024).
2. R Lucrezi, E Kogler, S Di Cataldo, M Aichhorn, L Boeri, C Heil, *Quantum lattice dynamics and their importance in ternary superhydride clathrates*, Communications Physics **6**, 298 (2023).
3. A. Sanna, C. Pellegrini, S. di Cataldo, G. Profeta and L. Boeri, *Possible explanation for the high superconducting Tc in bcc Ti at high pressure*, Phys. Rev. B **108**, 214523 (2023) – *Editor's Suggestion.*
4. P. P. Ferreira, L. J. Conway, A. Cucciari, S. Di Cataldo, F. Giannessi, E. Kogler, L. T. F. Eleno, C. J. Pickard, C. Heil and L. Boeri, *Search for ambient superconductivity in the Lu-N-H system*, Nature Comm. **14**, 5367 (2023) – *Editor's Suggestion.*
5. S. di Cataldo and L. Boeri, Phase diagram and superconductivity of Calcium Alanates under pressure, *J. Phys. Condens. Matter* **35** 445701 (2023).
6. S. Saha, S. Di Cataldo, F. Giannessi, A. Cucciari, W. von der Linden, and L. Boeri, *Mapping superconductivity in high-pressure hydrides: The Superhydra project*, Phys. Rev. Materials **7**, 054806 (2023).
7. S. Di Cataldo and L. Boeri, *Metal borohydrides as ambient-pressure high Tc superconductors***,** Phys. Rev. B **107**, L060501 (2023).
8. C. Tresca, G. Profeta, G. Marini, G.B. Bachelet, A. Sanna, M. Calandra, L. Boeri, *"Why Mercury is a superconductor",* Phys. Rev. B **106**, L180501 (2022) – APS highlight of the year 2022.
9. R. Lucrezi, S. di Cataldo, W. von der Linden, L. Boeri and Christoph Heil, *"In-silico synthesis of lowest-pressure high-Tc Superhydrides",* NPJ Computational Materials, **8**, 119 (2022).
10. S. di Cataldo, S. Qulaghasi, G. B. Bachelet, L. Boeri, *"High-T_c Superconductivity in doped boron-carbon clathrates"*, Phys. Rev. B **105**, 064516 (2022)
11. S. di Cataldo, W. Von der Linden, L. Boeri, *"First-principles search of hot superconductivity in La-X-H ternary hydrides",* Nature Partner Journal Computational Materials, **8**, 2 (2022).
12. S. Saha, W. von der Linden, and L. Boeri, "*Fused borophenes: A new family of superhard light-weight materials"*, Phys. Rev. Materials **5**, L080601 (2021).
13. S. Di Cataldo, C. Heil, W. von der Linden, and L. Boeri, *"LaBH8: Towards high-Tc low-pressure superconductivity in ternary superhydrides"*, Phys. Rev. B **104**, L020511 (2021).
14. S. Di Cataldo, Wolfgang von der Linden, and Lilia Boeri, "Phase diagram and superconductivity of calcium borohyrides at extreme pressures",Phys. Rev. B **102**, 014516 (2020).
15. S. Saha, S. Di Cataldo, M. Amsler, W. von der Linden, and L. Boeri, "High-temperature conventional superconductivity in the boron-carbon system: Material trends", Phys. Rev. B **102** 024519 (2020).
16. A. Smolyanyuk, M. Aichhorn, I.I. Mazin and L. Boeri, *Ab initio prediction of a two-dimensional variant of the iridate IrO2*, Phys. Rev. B **100**, 235114 (2019).

17. C. Heil, S. di Cataldo, G.B. Bachelet, L. Boeri, *"Superconductivity in sodalite-like yttrium hydride clathrates",* Phys. Rev. B **99**, 220502 (2019).
18. L. Boeri, G. B. Bachelet, "*The Road to Room-Temperature Superconductivity*", Journal of Physics Condensed Matter, **31**, 234002 (2019).
19. "*Absence of superconductivity in iron polyhydrides at high pressures*", Christoph Heil, Giovanni B. Bachelet, and Lilia Boeri, Phys. Rev. B **97**, 214510 (2018) – ***Editor's suggestion*.**
20. *"Ab initio study of ABiO3 (A=Ba, Sr, Ca) under high pressure*"**,** Andriy Smolyanyuk, Cesare Franchini, and Lilia Boeri, Phys. Rev. B **98**, 115158 (2018).
21. *"Lattice dynamics of the cluster chain compounds M2Mo6Se6 (M=K,Rb,Cs, In and Tl)"*, Liam Gannon, Lilia Boeri, Christopher A. Howard, Patrick Gougeon, Philippe Gall, Michel Potel, Diala Salloum, Alexander P. Petrović, and Moritz Hoesch, Phys. Rev. B **98**, 014104 (2018).
22. J. A. Flores-Livas, M. Graužinytė, L. Boeri, G. Profeta, A. Sanna, "*Superconductivity in doped polyethylene at high pressure*", European Physics Journal B, **91**, 176 (2018).
23. A. Smolyanyuk, L. Boeri, and C, Franchini, *Ab initio* prediction of the high- pressure phase diagram of BaBiO3, Phys. Rev. B **96**, 035103 (2017).
24. P.Chakraborty, T. Das, D. Nafday, L. Boeri, and T. Saha-Dasgupta, Manipulating the mechanical properties of Ti2C MXene: Effect of substitutional doping, Phys. Rev. B **95**, 184106 (2017),
25. C. Kokail, W. von der Linden, and L. Boeri, *Prediction of high-Tc conventional superconductivity in the ternary lithium borohydride system*, Phys. Rev. Materials **1**, 074803 (2017).
26. J. A. Flores-Livas, A. Sanna, A. P. Drozdov, L. Boeri, G. Profeta, M. Eremets, and S. Goedecker, *Interplay between structure and superconductivity: Metastable phases of phosphorus under pressure*, Phys. Rev. Materials **1**, 024802 (2017) - ***Editor's suggestion***.
27. M Rumetshofer, G. Dorn, L. Boeri, E Arrigoni and W von der Linden, *First- principles molecular transport calculation for the benzenedithiolate molecule*, New Journal of Physics,**19,** 103007 (2017).
28. "*A disorder-enhanced quasi-one-dimensional superconductor*", A.P. Petrović, D. Ansermet, D. Chernyshov, M. Hoesch, D. Salloum, P. Gougeon, M. Potel, L. Boeri, C. Panagopoulos, Nature Communications*, **7,** (2016);
29. "*Quasiparticle bands and structural phase transition of iron from Gutzwiller density-functional theory*", Tobias Schickling, Jörg Bünemann, Florian Gebhard, and Lilia Boeri, Phys. Rev. B **93**, 205151 (2016);
30. *"Reentrant Phase Coherence in Superconducting Nanowire Composites*", Diane Ansermet, Alexander P. Petrović, Shikun He, Dmitri Chernyshov, Moritz Hoesch, Diala Salloum, Patrick Gougeon, Michel Potel, Lilia Boeri, Ole Krogh Andersen, and Christos Panagopoulos, ACS Nano **10**, 515 (2016).
31. "*Search for high-Tc conventional superconductivity at megabar pressures in the lithium-sulfur system",* Christian Kokail, Christoph Heil, and Lilia Boeri, Phys. Rev. B **94**, 060502(R) (2016). ***(Editor's suggestion)***
32. "*Structural Evolution of Solid Phenanthrene at High Pressures*", F. Capitani, M. Höppner, L. Malavasi, C. Marini, G. A. Artioli, M. Hanfland, P. Dore, L. Boeri and P. Postorino, J. Phys. Chem. C, **120**, 14310 (2016).
33. "*Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure*", José A. Flores-Livas, Maximilian Amsler, Christoph Heil, Antonio Sanna, Lilia Boeri, Gianni Profeta, Chris Wolverton, Stefan Goedecker, and E. K. U. Gross, Phys. Rev. B **93**, 020508(R) (2016). *(**Editor's suggestion**).*
34. "*Influence of bonding on superconductivity in high-pressure hydrides*", Christoph Heil and Lilia Boeri, Phys. Rev. B **92**, 060508(R) (2015).
35. "*Structural origin of the anomalous temperature dependence of the local magnetic moments in the $CaFe_2As_2$ family of materials*", L. Ortenzi, H. Gretarsson, S. Kasahara, T. Shibauchi, K. D. Finkelstein, W. Wu, S.R. Julian, Young-June Kim, I. I. Mazin and L. Boeri, Phys. Rev. Lett. **114**, 047001 (2015).
36. "*Effect of the iron valence in the two types of layers in $LiFeO_2Fe_2Se_2$*", Christoph Heil, Lilia Boeri, Heinrich Sormann, Wolfgang von der Linden, Markus Aichhorn, Phys. Rev. B **90**, 165122 (2014).
37. "*Accurate bare susceptibilities from full-potential ab-initio calculations*", Christoph Heil, Heinrich Sormann, Lilia Boeri, Markus Aichhorn, Wolfgang von der Linden, Phys. Rev. B Phys. Rev. B **90**, 115143 (2014).
38. "*Single 20meV boson mode in KFe2As2 detected by point-contact spectroscopy*", Yu.G. Naidyuk, O.E.

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40. "*Combined experimental and computational study of the pressure dependence of the vibrational spectrum of solid picene C22H14*", F. Capitani, M. Höppner, B. Joseph, L. Malavasi, G. A. Artioli, L. Baldassarre, A. Perucchi, M. Piccinini, S. Lupi, P. Dore, L. Boeri, and P. Postorino, Phys. Rev. B **88**, 144303 (2013).
41. "*Electron-phonon superconductivity in APt3P (A=Sr, Ca, La) compounds: From weak to strong coupling*", Alaska Subedi, Luciano Ortenzi, and Lilia Boeri, Phys. Rev. B **87**, 144504 (2013).
42. "*Accounting for spin fluctuations beyond local spin density approximation in the density functional theory*", L. Ortenzi, I. I. Mazin, P. Blaha, and L. Boeri, Phys. Rev. B **86**, 064437 (2012).
43. "*Specific heat and upper critical fields in KFe2As2 single crystals*",M. Abdel-Hafiez, S. Aswartham, S. Wurmehl, V. Grinenko, C. Hess, S.-L. Drechsler, S. Johnston, A. U. B. Wolter, B. Büchner, H. Rosner, and L. Boeri, Phys. Rev. B **85**, 134533 (2012).
44. Erratum: "*Specific heat and upper critical fields in KFe2As2 single crystals*",M. Abdel-Hafiez, S. Aswartham, S. Wurmehl, V. Grinenko, C. Hess, S.-L. Drechsler, S. Johnston, A. U. B. Wolter, B. Büchner, H. Rosner, and L. Boeri, Phys. Rev. B **85**, 134533 (2012).
45. "*Anomalous dependence of c-axis polarized Fe B1g phonon mode with Fe and Se concentrations in Fe1+yTe1−xSex*", Y. J. Um, A. Subedi, P. Toulemonde, A. Y. Ganin, L. Boeri, M. Rahlenbeck, Y. Liu, C. T. Lin, S. J. E. Carlsson, A. Sulpice, M. J. Rosseinsky, B. Keimer, and M. Le Tacon Phys. Rev. B **85**, 064519 (2012).
46. *"Vibrational Spectrum of solid Picene (C22H14)",* B. Joseph, L. Boeri, L. Malavasi, F. Capitani, G.A. Artioli, S. Protti, M. Fagnoni, A. Albini, C. Marini, L. Baldassarre, A. Perucchi, S. Lupi, P.Postorino, P. Dore, Journal of Physics Condensed Matter **24**, 252203 (2012).
47. "*Gutzwiller Theory of Band Magnetism in LaOFeAs*", Tobias Schickling, Florian Gebhard, Jörg Bünemann, Lilia Boeri, Ole K. Andersen, and Werner Weber, Phys. Rev. Lett. **108**, 036406 (2012).
48. "*Vibrational spectrum and electron-phonon coupling of doped solid picene from first principles*", Alaska Subedi and Lilia Boeri, Phys. Rev. B **84**, 020508 (2011).
49. "*Extended Drude model and role of interband transitions in the midinfrared spectra of pnictides*", L. Benfatto, E. Cappelluti, L. Ortenzi, and L. Boeri, Phys. Rev. B **83**, 224514 (2011).
50. "*Competition between electron-phonon coupling and spin fluctuations in superconducting hole-doped CuBiSO*", Luciano Ortenzi, Silke Biermann, Ole Krogh Andersen, I. I. Mazin, and Lilia Boeri, Phys. Rev. B **83**, 100505 (2011).
51. "*Phonon mode spectroscopy, electron-phonon coupling, and the metal-insulator transition in quasi-one-dimensional M2Mo6Se6* ", A. P. Petrović, R. Lortz, G. Santi, M. Decroux, H. Monnard, Ø. Fischer, L. Boeri, O. K. Andersen, J. Kortus, D. Salloum, P. Gougeon, and M. Potel, Phys. Rev. B **82**, 235128 (2010). ***(Editor's suggestion)***
52. "*Effects of magnetism and doping on the electron-phonon coupling in BaFe2As2",* L. Boeri, M. Calandra, I.I. Mazin, O.V. Dolgov, F. Mauri, Phys. Rev. B **82**, 020506 (R), 2010. ***(Editor's suggestion)***
53. "*Problems with reconciling density functional theory calculations with experiement in ferropnictides"*, I.I. Mazin, M.D. Johannes, L. Boeri, K. Koepernik, D.J. Singh, Phys Rev. B, **78**, 085104 (2008). ***(Editor's suggestion)***
54. "*Is LaFeAsO1-xF_x an Electron-Phonon Superconductor?*", L. Boeri, O. V. Dolgov, and A. A. Golubov, Phys. Rev. Lett., **101**, 026403 (2008).
55. "*Optical properties of V1-xCr_xO_2 compounds under high pressure*", C. Marini, E. Arcangeletti, D. Di Castro, L. Baldassare, A. Perucchi, S. Lupi, L. Malavasi, L. Boeri, E. Pomjakushina, K. Conder, and P. Postorino, Phys. Rev. B, **77** , 235111 (2008).
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58. "*Electron-phonon interaction in Graphite Intercalation Compounds*", L. Boeri, G. B. Bachelet, M. Giantomassi, O. K. Andersen, Phys. Rev. B **76**, 064510 (2007).
59. *"Superconductivity in Heavy Alkaline-Earths Intercalated Graphites"*, J. S. Kim, L. Boeri, J. R. O'Brien, F. S. Razavi, R. K. Kremer, Phys. Rev. Lett. **99**, 027001 (2007). ***(Editor's suggestion)***
60. *"Linear Response separation of a solid into atomic constituents: Li, Al and their evolution under pressure",* J. Kunstmann, L.Boeri, W.E. Pickett, Phys. Rev. B **75**, 075107 (2007).
61. *"Effect of Pressure on Superconducting Ca-intercalated Graphite CaC6*", Kim J.S., L. Boeri, R. K. Kremer, F.S. Razavi, Phys. Rev. B **74**, 214513 (2006).
62. *"Momentum-Resolved Electron-Phonon Interaction in Lead Determined by Neutron Resonance Spin-Echo Spectroscopy",* Keller T., P. Aynajian, K. Habicht, L. Boeri, S.K. Bose, and B. Keimer, Phys. Rev. Lett. **96**, 225501 (2006).
63. *"Specific Heat of the Ca-Intercalated Graphite Superconductor CaC6",* Kim J.S., R. K. Kremer,L. Boeri, F.S. Razavi, Phys. Rev. Lett. **96**, 217002 (2006).
64. "*Electrons and phonons in the ternary alloy CaAl2-xSix as a function of composition*", M. Giantomassi, L. Boeri, G.B. Bachelet, Phys.Rev. B **72** , 224512 (2005).
65. "*Small Fermi energy, zero-point fluctuations, and nonadiabaticity in MgB2",* L. Boeri, E. Cappelluti, and L. Pietronero, Phys. Rev. B **71**, 012501 (2005).
66. *"Three-Dimensional MgB2-Type Superconductivity in Hole-Doped Diamond*", L. Boeri, J. Kortus, and O. K. Andersen, Phys. Rev. Lett. **93** 237002 (2004).
67. *"Poor Screening and non-adiabatic superconductivity in correlated systems*", L. Boeri, E. Cappelluti, C. Grimaldi, L. Pietronero, Phys. Rev. B **68** 214514 (2003).
68. *"Small Fermi energy and phonon anharmonicity in MgB2 and related compounds"*, L. Boeri, E. Cappelluti, G.B. Bachelet and L. Pietronero, Phys. Rev. B **65** 214501 (2002).

Invited Reviews (with Referee):

69. L. Boeri, O.V. Dolgov, A. A. Golubov, "*Electron Phonon Coupling of Pnictide Superconductors",* Physica C **469**, 628 (2009*)*.
70. O.K. Andersen and L. Boeri, *"On the multi-orbital band structure and itinerant magnetism of iron-based superconductors*", Annalen der Physik, **523**, 1 (2011). (this paper was also selected as a cover paper for the relaunch issue of Annalen der Physik in 2012).
71. J. A. Flores-Livas, L. Boeri, A. Sanna, G. Profeta, R. Arita, M. Eremets, "*A perspective on Conventional Superconductors at High Pressures: Methods and Materials*", Physics Reports **856**, 1-78 (2020).
72. L. Boeri, et al., *the 2021 Room-Temperature Superconductivity Roadmap*, Journal of Physics Condensed Matter **34**, 183002 (2022) *(Editor, together with R. Hennig, P. Hirschfeld, G. Profeta, A. Sanna, E. Zurek).*

Book Chapters

73. *"Understanding Novel Superconductors with Ab-Initio Calculations",* Springer Handbook of Material Modelling, Springer, (2018) – *Editors Sydney Yip, W. Andreoni.*

Conference Proceedings (with Referee):

74. L. Boeri, E. Cappelluti, C. Grimaldi, L.Pietronero, "*Effect of Strong Correlation on the Electron-Phonon Interaction* " Int. Journ. Mod. Phys. B, **14**, 2970, (2000).
75. L. Boeri, E. Cappelluti, G.B. Bachelet, L. Pietronero. "*The origin of phonon anharmonicity in MgB2 and related compounds*", Supercond. Sci. Technol. **16**, 143 (2003).
76. E. Cappelluti, C. Grimaldi, L. Pietronero, S. Straessler, L. Boeri, G.B. Bachelet, "*Non adiabatic effects and the role of small Fermi energy in MgB2*", International Journal of Modern Physics B, **17**, 560 (2003).
77. E. Cappelluti, G.B. Bachelet, L. Boeri, S. Ciuchi, C. Grimaldi, L. Pietronero and S. Strässler, "*Small Fermi energy effects in MgB2 and related compounds*", Physica C **332**, 408 (2004).
78. L. Boeri, J. Kortus, and O. K. Andersen, "*Electron-phonon superconductivity in hole-doped diamond: A*

first-principles study", Journ. of Physics and Chemistry of Solids **67**, 552 (2006).

79. L. Boeri , J. Kortus, O.K. Andersen "*Normal and Superconducting State Properties of B-doped diamond from First-Principles*", Sci. and Techn. of Adv. Mat., S54-S59 Sp. Iss. **1** (2006).
80. I.I. Mazin, L. Boeri, O.V. Dolgov, A.A. Golubov, G.B. Bachelet, M. Giantomassi and O.K. Andersen, "*Unresolved problems in superconductivity of CaC6*", Physica C **460** 116 (2007).
81. F. Capitani, M. Hoeppner, L. Malavasi, C. Marini, P. Dore, L. Boeri and P. Postorino, *The effect of high pressure on the lattice structure and dynamics of phenacenes*, Journal of Physics Conf. Series, **950**, 042017 (2017).
82. L. Pietronero, L. Boeri, L. Ortenzi, E. Cappelluti, *Conventional/unconventional superconductivity in high-pressure hydrides and beyond: insights from theory and perspectives*, Quantum Studies: Mathematics and Foundations **5**, 5 (2018).
83. F. Bernardini, L. Boeri, A. Floris, C. Franchini, G. Profeta, A. Sanna, "*Preface to the special issue on novel superconducting and magnetic materials*", Journal of Physics Condensed Matter 32, 040401 (2020).

Part XIV– Full List of Talks and Seminars (until August 2024):

1. ``*Piccoli valori dell'energia di Fermi e anarmonicita' dei fononi in MgB2 e materiali analoghi*", 24/3/**2002**, XXI Convegno di Fisica Teorica e Struttura della Materia, Fai della Paganella (TN), Italy
2. ``*Anharmonicity and non-adiabatic e-ph interaction in MgB2 and bad-actors superconductors*", 26/6/**2003**, VIII Convegno Nazionale di Fisica Statistica e dei Sistemi Complessi, Parma (Italy).
3. ``*Hole-doped Diamond: a 3D version of MgB2?*", at the "MPI-Stuttgart/Swedish Midsummer School, on Computational superconductivity.", Chalmers University, Goteborg, Sweden, June 23rd **2004**.
4. ``*Three-Dimensional MgB2-type superconductivity in hole-doped diamond*", DYPROSO 2005, 30th International Symposium on Dynamical Properties of Solids, Cesky Krumlov, Czech Republic, September 29th **2005**.
5. ``*Three-Dimensional MgB2-type superconductivity in hole-doped diamond*", IWSDRM2005, International Workshop on Superconductivity in Diamond and Related Materials, Tsukuba, Japan, December 8th **2005**.
6. ``*Electron-phonon Interaction in CaC6, a heavily e-doped graphite*", QCCM2006,Cambridge, UK, July 6th, **2006**.
7. ``*Understanding the electron-phonon interaction in s-p superconductors with first-principles calculations"*, Cancun, Mexico, August 23rd, **2006**.
8. ``*Superconductivity in Heavily Electron-Doped Graphite*", Lonavla, India, February **2007**.
9. ``*Nuovi Superconduttori Esagonali: Che cosa determina l'interazione elettrone-fonone?",* SATT 13, Porto Venere, Italy, 22-23 March **2007**.
10. ``*Electron-Phonon Interaction in Hexagonal Layered Compounds: Alkali-Earth Intercalated Graphites and Disilicides*", San Sebastian-Donostia, May 28-30, **2007**.
11. ``*Electron-Phonon Interaction in Hexagonal Layered Superconductors*", Workshop on Strongly Correlated Electron Systems, Ringberg Castle, Germany, 4-9 November **2007**.
12. ``*Electron-Phonon Superconductivity in Graphite Intercalation Compounds* ", SATT 14, 14th Italian Conference on High-Temperature Superconductivity, Parma, Italy 19th-21st March **2008**.
13. ``*Electronic and vibrational properties of Fe-based superconductors*", Meeting on Fe-based layered superconductors, Rome, Italy 14th May **2008**.
14. ``Electronic and vibrational properties of Fe-based superconductors",European Meeting on Road to Room Temperature Superconductivity, Bruxelles, Belgium, 20 May **2008**.
15. ``*Understanding the Electronic structure of Fe-As superconductors*", Joint Workshop of the MPI-FKF Stuttgart, Abteilungen Andersen, Keimer and Metzner, and the DFG Research Unit 538 Ringberg Castle, Germany, 3rd – 7th November, **2008**.
16. ``*Electron-phonon properties of FeAs superconductors*",``Superstripes 2008'', Rome, Italy,9th-13th December **2008**.
17. ``*DFT studies of Fe-As superconductors*", 14th "Total Energy" workshop, Trieste, Italy, 8-10 January **2009**.
18. ``*DFT studies of Fe-based superconductors*", PSI-K workshop, Alghero, Italy, September **2009**.
19. "*Magnetism and Superconductivity in exotic Superconductors*",
    CNR DMD school of Physics "Physics of Spin in Materials", November **2009**.
20. *"Electronic Structure of Fe pnictides and related compounds",*Workshop "Properties of high temperature superconductors", Munich, Germany, April **2010**.
21. "*Effect of magnetism on the electron-phonon properties of Fe pnictides*", joint Workshop of the MPI-FKF Stuttgart, Abteilungen Andersen, Keimer and Metzner, and the DFG Research Unit 538 Ringberg Castle, Germany, April, **2010**.
22. "*Effect of magnetism on the electron-phonon properties of Fe pnictides*", Topical Meeting on "Advanced First-Principles Calculations and Many-Body Effects in Correlated Electrons", Riken, Japan, September **2010**.
23. "*Iron-based superconductors, what can we learn from DFT?"*, PSIK 2010 conference, Berlin, September **2010**.

24. "*Electron-phonon interaction in Fe-based superconductors: what can we learn from DFT?*", Workshop on Electron-phonon interaction in metals, superconductors and semiconducting nanostructures", Paris, December **2010**.
25. "*Electronic Structure of Fe-based Superconductors: Magnetism and Electron-Phonon Interaction*", KITP Miniprogram: Iron-Based Superconductors, Santa Barbara, January **2011**.
26. 477. Heraeus-Seminar "Unconventional Superconductivity" in Bad Honnef, Germany, April 11-13, **2011**.
27. "*Doped Picene, a possible exotic electron-phonon superconductor*",Ringberg Symposium on High Temperature Superconductivity in Ringberg, 19th May **2011**)
28. "*Doped Picene, a possible exotic electron-phonon superconductor*"International Conference STRIPES11, Sapienza University of Rome, Rome, Italy from July 10 to July 16, **2011**.
29. **Keynote Speaker**, Spp 1458 Theory Meeting on Fe-based superconductors, Frankfurt (Germany), January **2012**.
30. *"Magnetism in Fe pnictides"*, Schloss Ringberg (Germany), November **2012**.
31. *"Superconductivity, A Computational Approach",* VICOM Meeting, April **2013.** (Vienna, Austria).
32. "*Electrons and Phonons in Intercalated Hydrocarbons", International Symposium on "Recent Electronic-Structure Theories and Related Experiments*", MPI Stuttgart, Germany, June **2013**.
33. "*Understanding Fe pnictides with DFT calculations*", 29th Panhellenic Conference on Solid State Physics and Materials Science, Athens, September **2013**.
34. "Electron-phonon superconductivity in AP3P compounds (A=Sr, Ca, La): From weak to strong coupling.", XXII Jahn-Teller Conference, TU Graz, August **2014**.
35. SuperFOX, Universita' la Sapienza, Roma, September **2014**.
36. Workshop "*Probing and Understanding Exotic Superconductors and Superfluids*", Trieste, Italy, 27-31 October **2014**.
37. "Electron-Phonon Interaction and Strong correlations", workshop on *Realistic Calculations for Correlated Electrons*, MPI Stuttgart, February **2015**.
38. "*Bonding, Electron-Phonon Interaction and Superconductivity in high-pressure hydrides",* General PSIK conference, San Sebastian-Donostia' (Spain), September **2015**.
39. "*High-pressure Hydrides: conventional high-Tc Superconductors",* Total Energy and Force Methods Conference, University of Luxembourg (Luxembourg), Jan. **2016**.
40. "*New Conventional High-Tc Superconductors*", 31. Obertraun Seminar on Superconductors and Novel Materials, Obertraun (Austria), Feb. **2016**.
41. "*High-T_c conventional superconductivity at extreme pressures*",", VICOM Meeting, Burg Schlaining, April **2016**.
42. *"High-Tc conventional superconductivity in high-Tc hydrides and related compounds",* International Workshop Superhydrides, CNR Roma, (Italy), May **2016**.
43. "*High-T_c conventional superconductivity at extreme pressures*", International Conference on Novel Spectroscopies, SNS 2016, Ludwisburg (Germany), June **2016**.
44. "*Designing novel transition metal oxides ab-initio*", (su invito), JSPS Core-to-Core Workshop on Novel Quantum and Functional Materials", MPI Stuttgart (Germania). **Aug 2017**
45. "*Robust Charge Density Wave Insulating State in ABiO3 Superconductors*" (su invito), SPP 1458 Final Workshop, presso IFW Dresden (Germania). **Feb 2018**
46. "*How to improve Superconducting High-Pressure Hydrides?*", RomeSC2018, Roma, Italy. **May 2018**
47. "*New surprises from high-pressure physics*", Workshop Lectiones Clitumnialae on correlated electrons, Umbria, Italy. **Aug. 2018**
48. "*Superconductivity Trends in High-Pressure Hydrides*", Gordon Research Conference on Superconductivity, Les Diablerets, Switzerland, **May 2019**.
49. "*High-Tc Conventional Superconductivity at High Pressure*", Conferenza SIF, l'Aquila, Italy, Sept. **2019.**
50. "*High-presssure Hydrides: to room temperature and beyond*", Paris Edge Workshop, France, Sept. **2019.**

51. "*Material Design con metodi computazionali e Big Data*", La Genesi dei Modelli: Teoria, Simulazione e Dati, *Accademia dei Lincei, 25-27* ***November 2019****.*
52. *"Ab-initio prediction of novel phases of Transition Metal Oxides"*, workshop on Novel Magnetic and Electronic Phases, Spin Center, Mainz, **December 2019.**
53. "*Near-Room-Temperature Superconductivity in High-Pressure Hydrides: A success story for ab-initio material Design*", Invited Talk at APS March Meeting, **2020** (The Meeting should have been held in Denver, Colorado, but was cancelled due to COVID; the presentation was uploaded on the Virtual March Meeting Platform.
54. "*Ab-initio design of new room-pressure Superconductors*", Invited talk at the APS March Meeting 2021, (online), March **2021** – The talk was also selected as a highlight for the APS Press conference.
55. *"Ab-initio design of new conventional Superconductors",* Invited Talk at the Workshop "Correlations in Novel Quantum Materials", MPI Stuttgart, 9-11 June **2021** (online).
56. M2S, 13th International Conference on Materials and Mechanisms for Superconductivity,Vancouver (Canada) **2022***.*
57. Workshop on the theory of condensed matter, Correlations in Novel Quantum Materials, June 20-23, **2022**, Stuttgart, Germany.
58. "*Ab-initio Design of Superconductors: how far is room temperature superconductivity?*", AIRAPT & EHPRG Conference, Edimburgh, UK, **July 2023**.
59. "*Ab-initio Design of Superconductors: how far is room temperature superconductivity?*", AIRAPT 16th European Conference on Applied Superconductivity (EUCAS), Bologna, **September 2023**.
60. Round Table on Room Temperature Superconductivity, 16th European Conference on Applied Superconductivity (EUCAS), **September 2023**.
61. *"Pressure-Induced High-Tc conventional Superconductivity*", APS March Meeting, Minneapolis, **March 2024**.
62. *"How close is Room-Temperature Superconductivity ?"* 8th IOP Summer School on Superconductivity, Oxford, UK, July 2024
63. *"Towards Low-Pressure High-Tc Conventional Superconductivity in Ternary Superhydrides",* Gordon Research Conference on High Pressure Physics, Holderness, USA, **July 2024**

Invited Seminars at National and International Universities and Research Centers

1. ``*Studio dell'origine dell'anarmonicità in MgB2 mediante DFT*", 17/5/**2002**, Centro ENEA Casaccia, Anguillara (Rome).
2. ``*Anharmonicity and Non-adiabaticity in MgB2 and A15*", 9/10/**2003**, Max-Planck Institute for Solid State Research, Stuttgart (Germany) (invited by J. Kortus).
3. ``*3D MgB2-like superconductivity in hole-doped diamond*", 17/5/**2004**, Max-Planck Institute for Solid State Research, Stuttgart (Germany)
4. ``*Electron-phonon Interaction in doped graphite Compounds*", 29/11/**2006**, Department of Mechanical Engineering and Materials Science, Duke University, Durham NC, USA, invited by S. Curtarolo.
5. ``*Superconductivity in Graphite-Intercalation Compounds*", 30/11/**2006**, Department of Physics, North Carolina State University, Rayleigh, NC (USA), invited by M. Buongiorno-Nardelli.
6. ``*Electron-Phonon Interaction in Hexagonal Layered Compounds: Alkali-Earth Intercalated Graphites and Disilicides*", Naval Research Lab, Washington DC, USA, **2007** (invited by Igor Mazin).
7. ``*Electron-Phonon Interaction in Alkali-Earth Intercalated Graphites*", Università Cattolica del Sacro Cuore, Brescia, Italy (invited by S. Pagliara), **2007**.
8. ``*Electron-Phonon Interaction in Alkali-Earth Intercalated Graphites*", Elettra, Trieste, Italy, **2008** (invited by F. Parmigiani).
9. *"Iron Superconductors, what can we learn from DFT?",* Material Modeling Lab, Oxford, UK, **2009** (invited by A. Kolmogorov), Kolloquium.
10. *"Iron Superconductors, what can we learn from DFT?", Universite' Pierre et Marie Curie*, Paris, France, **2009** (invited by M. Calandra).
11. ``*Higher-Tc superconductivity from Density Functional Calculations*", MPI-FKF, Stuttgart, **2009**.

12. *"Iron-based Superconductors, what can we learn from DFT?", TU Wien*, Vienna, Austria 25/1/2010 (invited by K.Held),**Kolloquium**.
13. *"Iron-based Superconductors, what can we learn from DFT?", KIT Karlsruhe*, Karlsruhe, Germany, 8/2/**2010** (invited by R. Heid), **Kolloquium**.
14. *"Iron-based Superconductors, new perspectives",Universita' di Roma la Sapienza,* Rome, Italy, June **2010***.*
15. *"Iron-based Superconductors, electron-phonon interaction", Naval Research Lab, Washington,* Jan **2011***.*
16. *"Iron-based Superconductors, new perspectives", University Marburg, Germany,* Feb 2011*.*
17. *"From doped semiconductors to pnictides: probing magnetic and superconducting properties with ab initio simulations", Institut Neel, Grenoble, France,* December **2011***.*
18. "*Understanding Superconductivity, First-Principles Calculations and beyond*", 23/5/2012, Technical Graz, Austria, June 2012.
19. "*Understanding Superconductivity, First-Principles Calculations and beyond*", Tu Wien, Austria, June **2012**.
20. "*Understanding Superconductivity from First-Principles Calculations*", University of Bristol (UK), June **2012**.
21. "*Carbon-based Superconductors*", 21/6/**2012**, University Marburg, **Kolloquium.**
22. "*Tuning Electron-Phonon Superconductivity in Pt Phosphides*", TU Dresden, January **2013**, **Kolloquium.**
23. *"Understanding superconductivity with first-principles calculations: from doped semiconductors to hydrocarbons", University Bochum, Germany*, April **2014**, **Kolloquium.**
24. *"Superconductivity in high-pressure hydrides", University Marburg, June **2015**, (Germany), **Kolloquium**.*
25. *"Ab-initio Calculations and Superconductivity", University Heidelberg (Germany), October **2015.***
26. *"Superconducting Hydrides", SNS Bose Center, Kolkata, India, March **2016**.*
27. *"High*-Tc conventional Superconductivity at extreme Pressures", University of *Wurzburg, Germany, **Kolloquium**, December **2016**,*
28. *"Superconduttori, Supercomputer e un puzzle che dura da 100 anni",* Seminario/lezione su invito presso il master in giornalismo scientifico della SISSA, Trieste - **Jan 2018:**
29. *"Searching for new high-temperature superconductors using high pressures and crystal structure prediction",* at Universita' della Florida, Gainesville, Usa - Host, Prof. P. J. Hirschfeld – ***Kolloquium*** - **Mar 2019.**
30. "*Ab-initio design of new high-Tc conventional superconductors*", Duke-CAMD/MURI/AFLOW seminar (online), **September 2021**.
31. "*Designing Superconductors with Supercomputers*", Symposium on Women in Condensed Matter Science, Max-Planck Institute Stuttgart, **February 2022.**
32. "*In-silico synthesis of new high-Tc Superconductors*", Seminar on Theoretical and Computational Physics, Graz University of Technology, **March 2022.**
33. *"Ab-initio Design of Superconductors, how far is Room-Temperature Superconductivity?",* Ames National Lab and Iowa State University (USA), **April 25, 2023**
34. *"Ab-initio Design of Superconductors, how far is Room-Temperature Superconductivity?",* NYSU Buffalo, USA, **April 27, 2023.**
35. *"Ab-initio Design of Superconductors, how far is Room-Temperature Superconductivity?"*– Kolloquium - MPI Stuttgart, Germany, **July 11th 2023.**