CURRICULUM VITAE
Dr. Raffaello Bianco

Personal details

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Research activity

I am a researcher in the field of theoretical and computational condensed matter physics. My research is characterized by the use of analytical and numerical techniques, in order to: develop new theoretical and algorithmic approaches to study the properties of materials from first-principles (*ab initio*); study fundamental theoretical questions; perform numerical simulations to interpret the results of experiments, explain a microscopic mechanism, or understand a general trend.
My scientific production stands out due to the variety of subjects studied, the diversity of methodologies employed, and for the novelty of the solutions proposed. I am coauthor of innovative concepts and methods in different fields of research (details below). I am the first author in the majority of my works and almost all the papers where I am not the first author are nonetheless works where the new methods developed by me are employed. The papers written by me stand out for the care adopted in describing with clarity and precision all the conceptual aspects of the conducted research. My current research interests include:

Phonon-phonon and electron-phonon interaction. Effects of anharmonicity
I am interested in studying the electron-phonon and phonon-phonon interactions, and their role in heat transfer, electronic transport, structural properties and phase transitions of materials. I study, in particular, the effects of anharmonicity in nonperturbative regime, an approach that is necessary whenever the system is close to a dynamical instability, light atoms are present, or temperature is high and the solid is not far from melting. I am coauthor of the theoretical development of a new method devised to predict and characterize displacive second order phase transitions and analyze phonon spectral properties of materials in presence of strong anharmonic effects, within the self-consistent harmonic approximation. I am also coauthor of a numerical implementation of this theory with a stochastic approach suited to be used in conjunction with first-principles calculations. Thus, the developed method allows to analyze ab initio the quantum anharmonic properties of materials at full nonperturbative level and, in particular, to calculate the critical temperatures for second-order structural phase transitions, and the phonon dispersions and spectra as a function of temperature. I am using this approach to the study, among others, the structural and electronic properties of transition metal dichalcogenides, ferroelectrics, superconducting hydrides, thermoelectrics. My current research interests include the development of theoretical and computational methods to study the non-perturbative effects that

anharmonicty has on the electron-phonon coupling and on carrier mobility. *I am one of the developers of the SSCHA code, a software devised to study quantum anharmonic effects at nonperturbative level in condensed matter systems. The code has been released to public at* http://sscha.eu/ .

Geometrical and topological effects on electronic properties

One of my poles of interest is the study of geometrical and topological effects in the electronic structure of materials. In particular, a fundamental theme in my research is the use of concepts as the geometric phase (Berry phase), the Berry curvature and the Chern number, in order to study a variety of arguments. Examples include the electronic polarization, the orbital magnetization, the electron transport and the anomalous Hall effect. I am the coauthor of a generalization, in the direct space, of the formula defining the Chern number in the reciprocal space of crystals. At variance with the original definition, this new formula is local in real space and is applicable to non-crystalline systems and molecules. In particular, it can be used to study the effect that disorder has on the topological properties, and to analyze the interfaces of heterojunctions between systems with different topological properties. I also used that new formulation of the Chern number to give, for the first time, a local expression for the orbital magnetization in real space. This has been used to unify the two different approaches used so far for finite-size systems (e.g. molecules) and crystals, and to clarify the role of surface states in topological insulators. I am also one of the developers of the "Berry curvature unfolding", a theoretical tool that can be used to study how the disorder affects the Berry phase contribution to the anomalous Hall conductivity. I have implemented this formulation by using Wannier functions in the Wannier90 code.

Education

20/03/2014 **Ph.D. in Physics**
Thesis: "*Chern Invariant and Orbital Magnetization as Local Quantities*"
Università di Trieste, Trieste, Italy
Supervisor: **Prof. Raffaele Resta**

24/03/2010 **"Laurea in Fisica" (Master degree in Physics)** (110/110 cum laude)
Thesis: "*Radiation propagation and cosmological observations in an Einstein-De Sitter universe with Lemaître-Tolman-Bondi spherical structures*"
Università degli Studi di Napoli "Federico II", Napoli, Italy
Supervisors : **Prof. G. Miele, Prof. G. Mangano**

Professional Experience

28/10/2022 – present **Assistant professor (RTD-B)**
Università degli Studi di Modena e Reggio Emilia (UNIMORE)
Modena, Italy

01/11/2021 – 27/10/2022 **Research associate (associate professor)**
Institute Ruder Boskovic (IRB)
Zagreb, Croatia

01/05/2019 – 31/10/2021 **Postdoctoral researcher**
Centro de Física de Materiales (CFM, CSIC-UPV/EHU)
San Sebastián-Donostia, Spain
Principal Investigator: **Prof. I. Errea**

16/04/2018 – 15/04/2019 **Postdoctoral researcher**
California Institute of Technology (CALTECH)
Department of Applied Physics and Materials Science,
Pasadena, California, USA
Principal Investigator: **Prof. M. Bernardi**

01/01/2017 – 31/03/2018 **Postdoctoral researcher**
Dipartimento di Fisica, Università di Roma "La Sapienza",
Istituto Italiano di Tecnologia (IIT)
Roma, Italy
Principal Investigator: **Prof. F. Mauri**

15/01/2014 – 31/12/2016 **Postdoctoral researcher**
Institut de mineralogie, de physique des materiaux et de cosmochimie (IMPMC),
Université Pierre et Marie Curie (UPMC) Paris VI, **CNRS**,
Paris, France
Principal Investigators: **Prof F. Mauri, Prof. M. Calandra**

Metrics (source Scopus)

Number of published papers: **26**

Number of citations: **1524**

H-Index: **19**

Academic Titles, Grants & Awards

2022 *Abilitazione Scientifica Nazionale* (ASN) alle funzioni di professore universitario di *Seconda Fascia* nel Settore Concorsuale 02/B2 – *Fisica teorica della materia* (qualification to have access to University associate professorship in Italy in condensed matter theory).

2020 *Six million hours of computation* with the Red Española de Supercomputación (RES) granted at the end of an evaluation process of a submitted research project.

2019 "*Seal of excellence*" certificate, delivered by the European Commission, in recognition of the high-quality level of the project proposal "*Towards a microscopic theory of Surface Polarization, Surface Orbital Magnetization, and Bulk Quadrupole Moments (SurfPolMag)*", submitted under the Horizon2020's *Marie Skłodowska-Curie actions*, call H2020-MSCA-IF-2018 of 12 September 2018.

2016 *Qualification à Maître de conférences, Condensed Matter section* (section 28) (qualification to conduct university teaching and to have access to University professorship in France).

Teaching and Tutoring Activities

2023 – present Professor of Physics I for the Faculty of Chemistry, University of Modena and Reggio Emilia

2021 - present PhD thesis co-direction with prof. Ion Errea for the student Josu Desu at Centro de Fisica de Materiales (CFM), San Sebastian, Pais Vasco, Spain.

2018 Collaboration with prof. Livia Bove and prof. Francesco Mauri in advising their master thesis student Francesco Lucantoni, Università di Roma "La Sapienza", Rome, Italy

2011 80 hours of teaching activity in Condensed Matter Physics for master students at International Centre for Theoretical Physics (ICTP), Trieste, Italy

Relevant Skills

Programming: Fortran 95, Python 2.7, Bash
Ab initio codes: Quantum Espresso, Wannier90, Crystal
Graphic and text: Matplotlib, Gnuplot, LATEX, Ipe, Xmgrace, Inkscape
Languages: Italian (native), English (excellent), French (intermediate)**Other**

Activities

Referee for Physical Review Letters, Physical Review B

Invited Talks

- **Ultrafast phenomena and light-matter interaction in quantum materials,** ***Ruđer Bošković Institute, Institute of Physics, University of Zadar,***
  Zadar, Croatia (2024)
  "*Theory of non-linear electron-phonon coupling and its first-principles implementation***"**

- **TDEP2023: Finite-temperature and anharmonic response properties of solids in theory and practice,**
  Linköping University, Linköping, Sweden (2023)
  "*Self-consistent phonons***"**

- **Electron-phonon coupling: Computational methods for electronic transport in nanostructures and in bulk materials**,
  CECAM, Lugano, Switzerland (2019)
  "*High-temperature superconducting hydrides: the crucial role of quantum anharmonic effects*"

- **Anharmonicity and thermal properties of solids**,
  CECAM, Paris, France (2018)
  "*Anharmonic phonons and second-order phase-transitions by the stochastic self-consistent harmonic approximation*"

- **Recent Developments in Electronic Structure Methods 2017**,
  Princeton University, Princeton, New Jersey, U.S. (2017)
  "*Anharmonic phonons and second-order phase-transitions by the stochastic self-consistent harmonic approximation*"

- **Trieste Quantum Days 2017**,
  SISSA, Trieste, Italy (2017)
  "*Orbital magnetization in insulators: Bulk versus surface*"

- **CFM**, San Sebastián, Spain (2015)
  "*Electronic and vibrational properties of $TiSe_2$ in the charge-density wave phase from first principles*"

- **CFM**, San Sebastián, Spain (2013)
  "*Orbital Magnetization as a Local Quantity*"

Organization of schools/workshops

- **SSCHA School 2023,** San Sebastian, Spain (2023)

Contributed Talks

- **Psi-k Conference 2022**, Lausanne, Switzerland (2022)
  "Theory of non-linear electron-phonon coupling and its first-principles implementation"

- **APS March Meeting 2019**, Boston, Massachusetts, USA (2019)
  "*Quantum enhancement of charge density wave in NbS_2 in the 2D limit*"

- **APS March Meeting 2013**, Baltimore, Maryland, USA (2013)
  "*Orbital Magnetization as a Local Quantity*"

Posters

- **Total Energy and Force Methods 2020**
  Donostia-San Sebastián, Spain (2020)
  "Quantum enhancement of charge density wave in NbS_2 in the 2D limit"

- **Psi-k Conference 2015**
  San Sebastián, Spain (2015)
  "*Electronic and vibrational properties of $TiSe_2$ in the charge-density wave phase from first principles"*

- 16th International Workshop on Computational Physics and Materials Science: **Total Energy and Force Methods**
  ICTP, Trieste, Italy (2013)
  "*Orbital Magnetization as a Local Quantity*"

- Workshop on Topological Insulators and Non-Perturbative Spin-Orbit Coupling
  CECAM-HQ-EPFL, Lausanne, Switzerland (2012)
  "*Mapping Topological Order on 'Haldanium' Samples*"

Publications

Where my name is marked with a (*), I am corresponding author.

[26] Đorđe Dangić, Lorenzo Monacelli, **Raffaello Bianco**, Francesco Mauri & Ion Errea
"*Large impact of phonon lineshapes on the superconductivity of solid hydrogen*"
Communications Physics, 7(1), 150 (2024)

[25] Jiabin Yu, Christopher J. Ciccarino, **Raffaello Bianco**, Ion Errea, Prineha Narang & B. Andrei Bernevig
"*Non-trivial quantum geometry and the strength of electron–phonon coupling*"
Nature Physics, 20(8), 1262 (2024)

[24] Unai Aseginolaza, Josu Diego, Tommaso Cea, **Raffaello Bianco**, Lorenzo Monacelli, Francesco Libbi, Matteo Calandra, Aitor Bergara, Francesco Mauri & Ion Errea
"*Bending rigidity, sound propagation and ripples in flat graphene*"
Nature Physics, 20, 1288 (2024)

[23] Diego, Josu and Subires, D. and Said, A. H. and Chaney, D. A. and Korshunov, A. and Garbarino, G. and Diekmann, F. and Mahatha, S. K. and Pardo, V. and Wilkinson, J. M. and Lord, J. S. and Strempfer, J. and Perez, Pablo J. Bereciartua and Francoual, S. and Popescu, C. and Tallarida, M. and Dai, J. and **Bianco, Raffaello** and Monacelli, Lorenzo and Calandra, Matteo and Bosak, A. and Mauri, Francesco and Rossnagel, K. and Fumega, Adolfo O. and Errea, Ion and Blanco-Canosa, S.
"*Electronic structure and lattice dynamics of $1T-VSe_2$: Origin of the three-dimensional charge density wave*"
Phys. Rev. B 109, 035133 (2024)

[22] Davide Romanin, Lorenzo Monacelli, **Raffaello Bianco**, Ion Errea, Francesco Mauri, and Matteo Calandra
"*Dominant Role of Quantum Anharmonicity in the Stability and Optical Properties of Infinite Linear Acetylenic Carbon Chains*"
J. Phys. Chem. Lett., 12,10339 (2021)

[21] Lorenzo Monacelli, **Raffaello Bianco***, Marco Cherubini, Matteo Calandra, Ion Errea, Francesco Mauri
"*The Stochastic Self-Consistent Harmonic Approximation: Calculating Vibrational Properties of Materials with Full Quantum and Anharmonic Effects*"
J. Phys.: Condens. Matter 33, 363001 (2021)

[20] Pugeng Hou, Francesco Belli, **Raffaello Bianco**, Ion Errea
"*Quantum anharmonic enhancement of superconductivity in $P6_3/mmc$ ScH_6 at high pressures: A first-principles study*"
J. Appl. Phys. 130, 175902 (2021)

[19] Pugeng Hou, Francesco Belli, **Raffaello Bianco**, Ion Errea
"*Strong Anharmonic and Quantum Effects in Pm-3n AlH3 Under High Pressure: A First-Principles Study*"
Phys. Rev. B 103, 134305 (2021)

[18] Josu Diego, A. H. Said, S. K. Mahatha, **Raffaello Bianco**, Lorenzo Monacelli, Matteo Calandra, Francesco Mauri, K. Rossnagel, Ion Errea, S. Blanco-Canosa
"*Phonon collapse and van der Waals melting of the 3D charge density wave of VSe_2*"
Nature Communications 12, 598 (2021)

[17] Ivan A. Troyan, Dmitrii V. Semenok, Alexander G. Kvashnin, Andrey V. Sadakov, Oleg A. Sobolevskiy, Vladimir M. Pudalov, Anna G. Ivanova, Vitali B. Prakapenka, Eran Greenberg, Alexander G.Gavriliuk, Viktor V. Struzhkin, Aitor Bergara, Ion Errea, **Raffaello Bianco**, Matteo Calandra, Francesco Mauri, Lorenzo Monacelli, Ryosuke Akashi, Artem R. Oganov
"*Anomalous high-temperature superconductivity in YH_6*"
Advanced Materials 33, 2006832 (2021)

[16] **Raffaello Bianco***, Lorenzo Monacelli, Francesco Mauri, Matteo Calandra, Ion Errea
"W*eak Dimensionality Dependence and Dominant Role of Ionic Fluctuations in the Charge-Density-Wave Transition of $NbSe_2$*"
Phys. Rev. Lett. 125, 106101 (2020)

[15] Jianqiang Sky Zhou, **Raffaello Bianco**, Lorenzo Monacelli, Ion Errea, Francesco Mauri, Matteo Calandra
"*Theory of the thickness dependence of the charge density wave transition in 1T-$TiTe_2$*"
2D Materials 7, 045032 (2020)

[14] Jianqiang Sky Zhou, Lorenzo Monacelli, **Raffaello Bianco**, Ion Errea, Francesco Mauri, Matteo Calandra
"*Anharmonicity and Doping Melt the Charge Density Wave in Single-Layer $TiSe_2$*"
Nano Lett. 20, 4809 (2020)

[13] Ion Errea, Francesco Belli, Lorenzo Monacelli, Antonio Sanna, Takashi Koretsune, Terumasa Tadano, **Raffaello Bianco,** Matteo Calandra, Ryotaro Arita, Francesco Mauri, José A. Flores-Livas
"*Quantum crystal structure in the 250-kelvin superconducting lanthanum hydride*"
Nature 578, 66 (2020)

[12] Unai Aseginolaza, **Raffaello Bianco**, Lorenzo Monacelli, Lorenzo Paulatto, Matteo Calandra, Francesco Mauri, Aitor Bergara, Ion Errea
"*Strong anharmonicity and high thermoelectric efficiency in high temperature SnS from first-principles*"
Phys. Rev. B 100, 214307 (2019)

[11] **Raffaello Bianco***, Ion Errea, Lorenzo Monacelli, Matteo Calandra, Francesco Mauri
"*Quantum enhancement of charge density wave in NbS_2 in the 2D limit*"
Nano Lett. 19, 3098 (2019)

[10] Unai Aseginolaza, **Raffaello Bianco**, Lorenzo Monacelli, Lorenzo Paulatto, Matteo Calandra, Francesco Mauri, Aitor Bergara, Ion Errea
"*Phonon Collapse and Second-Order Phase Transition in Thermoelectric SnSe*"
Phys. Rev. Lett. 122, 075901 (2019)

[9] **Raffaello Bianco***, Ion Errea, Matteo Calandra, Francesco Mauri
"*High-pressure hydrogen sulfide from first principles: quantum hydrogen-bond symmetrization, isotope effect, anharmonic phonon frequencies and phonon spectra*"
Phys. Rev. B 97, 214101 (2018)

[8] Guilherme A. S. Ribeiro, Lorenzo Paulatto, **Raffaello Bianco**, Ion Errea Matteo, Calandra, Francesco Mauri
"*Strong anharmonicity in the phonon spectra of PbTe and SnTe from first principles*"
Phys. Rev. B 97, 014306 (2018)

[7] Maria Hellgren, Jacopo Baima, **Raffaello Bianco**, Matteo Calandra, Francesco Mauri, Ludger Wirtz
"*Critical role of exchange interaction for the electronic structure and charge-denisty-wave formation in $TiSe_2$*"
Phys. Rev. Lett. 119, 176401 (2017)

[6] **Raffaello Bianco***, Ion Errea, Lorenzo Paulatto, Matteo Calandra, Francesco Mauri
"*Second order structural phase transitions, free energy curvature, and temperature-dependent anharmonic phonons in the self-consistent harmonic approximation : theory and stochastic implementation*"
Phys. Rev. B 96, 014111 (2017)

[5] **Raffaello Bianco**, Raffaele Resta
"*Orbital magnetization in insulators : Bulk versus surface*"
Phys. Rev. B 93, 174417 (2016)

[4] **Raffaello Bianco***, Matteo Calandra, Francesco Mauri
"*Electronic and vibrational properties of TiSe2 in the charge-density wave phase from first principles*"
Phys. Rev. B 92, 094107 (2015)

[3] **Raffaello Bianco**, Raffaele Resta, Ivo Souza
"*How disorder affects the Berry-phase anomalous Hall conductivity : A reciprocal-space analysis*"
Phys. Rev. B 90, 125153 (2014)

[2] **Raffaello Bianco**, Raffaele Resta
"*Orbital magnetization as a local property*"
Phys. Rev. Lett. 110, 087202 (2013)

[1] **Raffaello Bianco**, Raffaele Resta
"*Mapping topological order in coordinate space*"
Phys. Rev. B 84, 241106 (2011)