

Curriculum vitae of Feliciano Giustino

Primary ERC subfields (max 3): *PE3_4 Electronic properties of materials, surfaces, interfaces, nanostructures; PE3_3 Transport properties of condensed matter; PE3_2 Mechanical and acoustical properties of condensed matter, lattice dynamics*

Secondary ERC subfields (max 3): *PE3_6 Macroscopic quantum phenomena (e.g. superconductivity); PE3_5 Physical properties of semiconductors and insulators; PE11_14 Computational methods for materials engineering*

PERSONAL DETAILS

Family name, First name: Giustino, Feliciano

Address: The University of Texas at Austin, Oden Institute for Computational Engineering and Sciences, 201 E 24th St, Austin, TX 78712, USA

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Education and key qualifications

2005 Ph.D. in Physics, École Polytechnique Fédérale de Lausanne (EPFL), Switzerland

2001 M.Sc. in Nuclear Engineering, Politecnico di Torino, Italy

Current position(s)

2019-present W. A. “Tex” Moncrief, Jr. Chair of Quantum Materials Engineering; Professor of Physics; Principal Faculty Member, Oden Institute for Computational Engineering and Sciences, The University of Texas at Austin, USA

Previous position(s)

2017-2018 Mary Shepard B. Upson Visiting Professor in Engineering, Cornell University, USA

2008-2019 Faculty, Department of Materials, University of Oxford, UK (Assistant Professor 2008-2013; Associate Professor 2013-2014; Professor 2014-2019)

2005-2008 Postdoctoral Researcher, Department of Physics, University of California at Berkeley, USA

2000-2001 Research Fellow, Experimental Physics Division, CERN, Switzerland

RESEARCH ACHIEVEMENTS AND PEER RECOGNITION

Research achievements

Profile and bibliometrics. Computational condensed-matter physicist specializing in electronic-structure theory, many-body methods, high-performance computing, and quantum materials design. Author of 205 journal articles, including 25 papers in Nature/Science journals or PNAS and 27 in Physical Review Letters, plus one monograph. Google Scholar h-index 79 and 45,000+ citations.

- 1. Wannier–Fourier interpolation of electron–phonon interactions.** *F. Giustino, M. L. Cohen, and S. G. Louie, Phys. Rev. B 76, 165108 (2007).* Introduced a localized Wannier representation and efficient Fourier interpolation strategy that made dense, parameter-free first-principles calculations of electron–phonon couplings practical for real materials. This approach became a standard foundation for modern calculations of transport, spectroscopy, and superconductivity.
- 2. EPW open-source software and exascale computing.** *S. Poncé et al., Comput. Phys. Commun. 209, 116 (2016); H. Lee et al., npj Comput. Mater. 9, 156 (2023); T. Y. Kim et al., npj Comput. Mater. 12, 199 (2026).* Founder and coordinator of EPW, the open-source software project for first-principles electron–phonon calculations. EPW has 800+ registered users and has been used in 1,800+ scientific papers. Recent work extended the same computational framework to scalable hybrid MPI–GPU–OpenMP execution for leadership-class systems.
- 3. Syntheses of electron–phonon and polaron physics.** *F. Giustino, Rev. Mod. Phys. 89, 015003 (2017); Z. Dai, J. Lafuente-Bartolomé, and F. Giustino, Rev. Mod. Phys. (2026), in press.* The 2017 single-author review consolidated the first-principles theory of electron–phonon interactions and has received more than 1,500 citations. The 2026 review outlines the modern first-principles framework for polarons, connecting model concepts to predictive calculations in real materials.
- 4. Ab initio theory of polarons beyond supercells.** *W. H. Sio et al., Phys. Rev. Lett. 122, 246403 (2019); J. Lafuente-Bartolomé et al., Phys. Rev. Lett. 129, 076402 (2022).* Co-developed a supercell-free, first-principles framework for polarons and a unified treatment connecting polaron formation with phonon-induced band renormalization across weak and strong coupling regimes.
- 5. Polarons in low dimensions and topological polaron states.** *W.-H. Sio and F. Giustino, Nat. Phys. 19, 629 (2023); J. Lafuente-Bartolomé et al., PNAS 121, e2318151121 (2024); Z. Dai and F. Giustino, PNAS 121, e2414203121 (2024); K. Luo et al., PNAS 123, e2514647123 (2026).* Extended the ab initio polaron framework to two-dimensional crystals and realistic oxides, and identified topological and symmetry-protected polaron states.
- 6. Excitonic polarons from first principles.** *Z. Dai, C. Lian, J. Lafuente-Bartolomé, and F. Giustino, Phys. Rev. Lett. 132, 036902 (2024).* Extended first-principles electron–phonon methods to coupled exciton–lattice quasiparticles, providing a route to calculate excitonic polarons and self-trapped excitons from microscopic exciton–phonon interactions.

- 7. Lead-free halide double perovskites and technology transfer.** *G. Volonakis et al., J. Phys. Chem. Lett.* 7, 1254 (2016); *G. Volonakis et al., J. Phys. Chem. Lett.* 8, 772 (2017); *licensed U.S., E.U., and China patent families on double perovskites*. Spearheaded a computational design strategy replacing lead by heterovalent cation pairs, helping establish lead-free halide double perovskites as a new semiconductor family. Co-inventor on related international patents that have been granted and licensed.
- 8. Predictive carrier transport and semiconductor engineering.** *S. Ponc , D. Jena, and F. Giustino, Phys. Rev. Lett.* 123, 096602 (2019); *C. F. C. Chang et al., Nat. Electron.* 9, 346 (2026); *N. Pant, S. Tiwari, S. G. Louie, and F. Giustino, Phys. Rev. Lett.* 137, 056303 (2026). Developed strategies for achieving high hole mobility in wide-gap semiconductors and contributed to a theory-experiment program on high-mobility holes in GaN. Recent work raised first-principles mobility prediction accuracy by incorporating GW perturbation theory for electron-phonon coupling.
- 9. Monograph on density-functional theory.** *F. Giustino, Materials Modelling Using Density Functional Theory: Properties and Predictions, Oxford University Press (2014)*. Single-author textbook presenting a unified, practical treatment of density-functional theory and first-principles materials modelling; it has become a widely cited reference for researchers and graduate students.

Peer recognition

- 2025 Guggenheim Fellow in Physics, Centennial Class.
- Clarivate Highly Cited Researcher for seven consecutive years (2019–2025).
- 2020 Fellow of the American Physical Society, cited “for pioneering contributions to the ab initio theory of electron-phonon interactions and its application to the electronic, optical, transport, and superconducting properties of solids”.
- 2023 Moncrief Grand Challenge Award, The University of Texas at Austin; 2012 Leverhulme Research Leadership Award; 2009 ERC Starting Grant.
- 172 invited talks, including 9 plenary and keynote talks.

ADDITIONAL INFORMATION

Other contributions to the research community

- **Research and software leadership:** founder of the EPW software project; institutional member of the Quantum ESPRESSO Foundation since 2017; lead PI of U.S. DOE and NSF programs on interoperable many-body software.
- **Leadership-class computing:** member of the NSF/TACC Characteristic Science Applications program for the upcoming Horizon system.
- **Advanced training:** lead organizer or co-organizer of recurrent international schools on electron–phonon physics and many-body perturbation theory. Recent editions include UT Austin 2024 and ICTP Trieste 2026.
- **Community leadership:** lead of Psi-k Working Group A2 on Perturbative Many-Body Methods (since 2024), member of the Psi-k Scientific Advisory Committee (since 2018), Scientific Advisory Board member of the Total Energies and Forces conference series, and Executive Committee member of the SRC JUMP 2.0 SUPREME Center.
- **Conference leadership:** organizer or co-organizer of international meetings spanning many-body electronic structure, electron–phonon physics, charge and heat transport, and computational physics, including symposia at Psi-k 2022 and 2025 and the 33rd IUPAP Conference on Computational Physics (2022).
- **National and international service:** member of the 2022 National Academies committee advising NSF on the Materials Genome Initiative; invited NSF panelist and reviewer, DOE ALCC reviewer, MRSEC reviewer.
- **Editorial service:** Associate Editor, *Journal of Computational Electronics* (2024–2026); Executive Editorial Board, *JPhys Materials* (2021–2026); former Associate Editor, *Computational Materials Science* (2015–2018) and *European Physical Journal B* (2012–2016).
- **Industry and translation:** materials consultant for Oxford Photovoltaics Ltd (2016–2019); co-inventor on licensed international patent families for lead-free double perovskites and on a pending patent application for automated generation of Wannier functions.

Career breaks, diverse career paths and major life events

None.