MARCO BUONGIORNO NARDELLI – SCIENCE CV

Regents Professor
Department of Physics, College of Science, and
Division of Composition Studies, College of Music
CEMI, Center for Experimental Music and Intermedia
iARTA, initiative for Advanced Research in Technology and the Arts
Center for Nonlinear Sciences
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MAIN RESEARCH INTERESTS

Computational materials and high-performance simulations, with particular emphasis on theoretical developments of ab initio DFT-based methods; high-throughput computational techniques and computational materials design; sustainable development of scientific software for high-performance materials simulations; novel algorithms for materials simulations on quantum computers; network theory and complexity science.

EDUCATION

1993 Ph.D. in Physics at the ``International School for Advanced Studies'' (SISSA/ISAS) in Trieste, Italy, under the supervision of Prof. S. Baroni.

1991 M.Sc. in Physics at the ``International School for Advanced Studies'' (SISSA/ISAS) in Trieste, Italy, under the supervision of Prof. S. Baroni.

1989 Degree (Laurea) in Physics summa cum laude at the University of Rome ``La Sapienza'' under the supervision of Prof. C.M. Bertoni and Prof. G. Ciccotti.

PROFESSIONAL EXPERIENCE

June 2023 to present	Regents Professor of Physics and Composition, University of North Texas
Feb. 2022 to June 2023	Regents Professor, University of North Texas
Aug. 2021 to present	External Faculty and leader of the working group on “Music Complexity and Structure”, Santa Fe Institute
Aug. 2021 to present	Faculty Member, Center for Nonlinear Sciences, College of Science, University of North Texas
Aug. 2019 to June 2023	Affiliated Faculty, Division of Composition Studies, College of Music, University of North Texas

July 2019-2020	Associate Fellow, IMéRA, Institute for Advanced Studies of Aix-Marseille University, Marseille, France
Sep. 2017 to present	Faculty member, CEMI, the Center for Experimental Music and Intermedia
Sep. 2015 to present	Faculty member, iARTA, initiative for Advanced Research in Technology and the Arts
Sep. 2014 to present	"University Distinguished Research" Professor, Department of Physics and Department of Chemistry, University of North Texas
Jan. 2012 to present	Full Professor, Department of Physics and Department of Chemistry, University of North Texas, Joint Faculty Appointment, ORNL
Aug. 2009 – Jan. 2012	Full Professor, Department of Physics, North Carolina State University, Joint Faculty Appointment, ORNL
Aug. 2005 – Aug. 2009	Associate professor, Department of Physics, North Carolina State University, Joint Faculty Appointment, ORNL
Aug. 2001 – Aug. 2005	Assistant professor, Department of Physics, North Carolina State University, Joint Faculty Appointment, ORNL
Nov. 1998 – Aug. 2001	Research associate, Department of Physics, North Carolina State University; group of Prof. J. Bernholc.
Nov. 1995 – Nov. 1998	Postdoc, Department of Physics, North Carolina State University; advisor: Prof. J. Bernholc.
Nov. 1993 – Nov. 1995	Postdoc, Laboratorio INFM/TASC (Advanced Technology in Surface Science and Catalysis), Trieste, Italy, in a joint theoretical-experimental project on ``Electronic structure calculations of semiconductor micro-structures, surfaces and interfaces'': advisor Prof. F. Tommasini.
Nov. 1994 – Nov. 1995	Lecturer, Department of Physics, University of Trieste, course: ``Modern methods in electronic structure theory'' (graduate level).
Jan. 1995 - Jul. 1995	Postdoc, ``Laboratoire de Recherches sur les Materiaux dans leur Environnement'', Université de Marne-la-Vallée, Paris, France; advisor: Prof. P. Cortona.

HONORS AND AWARDS

- Associate Editor, Advances in Complex Systems (World Scientific), 2024-present
- External Faculty, Santa Fe Institute, 2021-present
- Associate Fellow, IMéRA, Institute for Advanced Studies of Aix-Marseille University, 2019
- Research Leadership Award, 2017
- University Distinguished Research Professor, 2014
- Member, Editorial Board, Scientific Reports (Nature Publishing Group), 2013.
- Fellow of the Institute of Physics, 2011.
- Fellow of the American Physical Society, 2010.

- Top Italian Scientists list (rank 100) from VIA-Academy: http://www.topitalianscientists.org/Top_italian_scientists_VIA-Academy.aspx.
- Member at large, User Executive Committee of the Center for Nanoscale Materials Sciences (CNMS), 2011-2012.
- Co-Chair, Symposium CCC: Integrating Experiments, Simulations and Machine Learning to Accelerate Materials Innovation, MRS Fall Meeting, 2015.
- Co-Chair, Symposium II "Theory and Computer Simulation of Materials", XIX International Materials Research Congress, Cancún, México, August 14-18, 2010
- Co-Chair, Symposium II "Theory and Computer Simulation of Materials", XVIII International Materials Research Congress, Cancún, México, August 18-22, 2009
- Chair, invited session on "Computational Science", SESAPS Meeting, Nashville, TN, November 2007
- Chair, DMP invited session on "Recent advances in the computation of optical and transport properties of nanostructures", APS March Meeting, Baltimore, MD, March 2006
- Chair, DMP focus session on "Computational Nanoscience", APS March Meeting, Baltimore, MD, March 2006
- Chair, DMP focus session on "Theory of dielectrics, piezoelectrics and multiferroics", APS March Meeting, Los Angeles, CA, March 2005.
- Sigma Xi Faculty Research Award, NCSU Chapter, May 2004.
- Member, Proposal Review Committee, Center for Nanophase Materials Sciences (CNMS), Oak Ridge National Laboratory
- Chair, DCOMP/DMP focus session on "Theory of Nanotubes", APS March Meeting, Austin, TX, March 3-7, 2003.
- Faculty Research and Professional Development Award, North Carolina State University, $4,000, 2003.
- First Annual North Carolina State University International Research Exposition Award in recognition of ``Outstanding Research in Physics'', Raleigh, April 16, 1999.

PATENTS AND INVENTIONS

- "BN/C nanotubes for Micro-Electro-Mechanical (MEM) applications", M. Buongiorno Nardelli, NCSU # 000-133, June 2000.
- "Coulomb Buffer as a Method for Adjusting Band Offset and Alignment at Semiconductor/Insulator and Semiconductor/Semiconductor Interfaces", F. Walker, R. Mc Kee, M. Buongiorno Nardelli, W.J. Shelton and M.G. Stocks, ORNL #1037, January 2002.
- "Piezoelectric and pyroelectric polymers with boron nitride backbone", S. Nakhmanson, M. Buongiorno Nardelli and J. Bernholc, NCSU #04-011, August 2003.

PUBLIC SCIENTIFIC SOFTWARE RELEASES

- PAOFLOW, A utility to construct and operate on ab initio Hamiltonians from the Projections of electronic wavefunctions on Atomic Orbital bases, including characterization of topological materials.

- MUSICNTWRK, A python library for pitch class set and rhythmic sequences classification and manipulation, the generation of networks in generalized music and sound spaces, deep learning algorithms for timbre recognition, and the sonification of arbitrary data
- AFLOWπ, a python platform for advanced high-throughput electronic structure simulations.
- AFLOWLIB.org, a distributed materials properties repository from high-throughput ab initio calculations.
- Quantum-ESPRESSO, www.quantum-espresso.org
- WanT, http://qe-forge.org/projects/want/, an integrated approach to ab initio electronic transport from maximally-localized Wannier functions, distributed as part of Quantum ESPRESSO.
- DOSQC_1.0, electronic transport properties of nanostructures from Tight-Binding Hamiltonians, available upon request at http://ermes.unt.edu.

SERVICE TO THE DEPARTMENT, COLLEGE AND UNIVERSITY

Department: executive committee, personnel action committee, graduate committee, equity diversity and inclusion committee (chair), search committees (chair), research roadmap committee (ad hoc), award committee, chair and member of numerous search committee;
College: personnel action committee, research roadmap committee (ad hoc)
University: Planning & Implementation Committee for Computational Science & Analytics, a2ru committee, innovation committee, AI Strategic Committee, COI committee.

STUDENTS AND POST-DOC MENTORED

Post-doc
Jagoda Slawinska, Priya Gopal, Ilaria Siloi, Laalitha Lyanage, Luis Agapito, Jeevaka Weerasinghe, Vivek Ranjan, Thushari Jayasekera, Matias Nunez, Liping Huang, Gunn Kim, Aaron M. George, Milen Kostov, Qingzhong Zhao, Serge Nakhmanson

Graduate students (current)*
UNT: Benjamin Shirey*, Colin Stokes*, Matthew Alltrock, Franklin Talbert, Jacob Owen, Anooja Jayaraj, Kyle Sherbert. Haihang Wang, Frank Cerasoli
NCSU: Rui Dong, Yifeng Chen, Shu Xu, Jeff Mullen, Sujata Paul, Liping Yu, Mandayan Krishnan, Matias Nunez, Erik Santiso

Undergraduate students (current)*
UNT: Jonathan Red*, William Medlar, Cristina Castillo, Jacob Callaway, Harvey Shi (TAMS student), Keisha McCall (REU summer student), Kara Beharry (REU summer student)

CURRICULAR MATERIAL DEVELOPMENT AND COURSES TAUGHT

- MUCP 4690/5690 “Coding Music: Computational Approaches to Music Creation”
- PHYS 5610 “Artificial Intelligence and Machine Learning for Scientists”
- MUCP 5690 “Generative Deep Learning for Music and Visuals”

- MUCP 6910 “Methods and esthetics of data sonification”, UNT Division of Composition Studies, Spring 2022.
- MUCP 4600-5700 “Generative and algorithmic composition in Python”, UNT Division of Composition Studies, Fall 2021.
- Various graduate seminars and special problem courses on computer music, algorithmic composition, and advanced music theory (2018 – present).
- PHYS 4500/5600 – “Advanced Computational Physics”, Spring 2018, Fall 2019, Fall 2020, 2021
- PHYS 6800- "Computational Physics of Materials", Fall 2014, 2015, 2016, 2018; Spring 2021
- PHYS 5450- “Solid State Physics”, Spring 2013, 2014
- PHYS 3210 – “Analytical Mechanics”, Fall 2012.
- PY 810 “Quantum many-body theory of materials” (new course, Fall 2008)
- HON 321 "Music and the Science of Sound" (Fall 2007, 2008, 2009, 2010, 2011, co-taught with Dr. Phill Stiles)
- PY 615 "Computational Physics of Materials" (new course, Spring 2006, 2007, 2008, 2009,2010, 2011)
- PY 205-208 "Physics for Scientists and Engineers" (Spring 2002, Spring 2003, Spring 2004, Spring 2005)
- PY610 "Modeling from the nanoscale to the macroscale" (Fall 2004)

RESEARCH GRANTS

Past

- PI: UT-Battelle-ORNL – joint faculty appointment, “Research and development in high performance computing and computational nanoscale science”, $53,275/year, 8/16/2001 – 30/10/2010.
- PI: American Chemical Society – Petroleum Research Fund (ACS-PRF) research grant – type G, “Ab initio Theory of Electronic Transport in Carbon Nanotubes and Nanotube-based Structures”, $37,500.00, 9/1/2002 – 9/1/2004.
- co-PI: NSF – NIRT (Nanoscale Interdisciplinary Research Team) program: “Reduced Degree of Freedom Predictive Methods for Control and Design of Interfaces in Nanofeatured Systems: Nanocrystalline Materials, Sensors and Composites”, $100,000/year , July 2003-July 2009.
- co_PI: DoE – Office of Science – NSET: “Integrated Multiscale Modeling in Molecular Computing Devices”, PI’s M. Buongiorno Nardelli, J. Bernholc, $230,000/year (2005-2011).
- co-PI: ORNL-SEED - "Real Space Imaging of High Frequency Transport on the Nanoscale." PI’s S. Kalinin, V. Meunier, A. P. Baddorf, M. Buongiorno Nardelli and D. B. Geohegan, $100,000 for one year (2004).
- PI: National Science Foundation-STC for Environmentally Responsible Solvents and Processes - $40,000 (2006-2007).
- co_PI: US Navy-Office of Naval Research - “Microscopic, macroscopic and multi-scale modeling of capacitor dielectrics and composites”, PIs: M. Buongiorno nardelli and J. Bernholc, $480,000, (2005-2011).

- co-PI: National Science Foundation - " Spin Dynamics and Device Applications in Carbon Nanotubes", PIs M. Buongiorno Nardelli and K.W. Kim, $441,151 (2006-2009).
- co-PI: NIST - Univ. of Texas - "Nanoscale Phonon Transport for Thermal Management", PI: Ki Wook Kim, 04/08-03-09.
- co-PI: DARPA-CERA - 2008-2011, $120K for phase I (18 months) and another approx. $120K for phase II (18 months).
- co-PI: NSF-CCI "Center for Molecular Spintronics", $120K for phase I (36 months).
- PI: ARO-DURIP – 2010, First principles calculations of electronic and phononic transport: a practical tool-set for efficient design of novel materials and devices for nanoelectronic applications", $67K.
- PI: SRC-CEMPI - Thermal Transport In Nanoscale Materials And Interfaces, 2013, $33,000
- co_PI: US Navy-Office of Naval Research - "Microscopic, macroscopic and multi-scale modeling of capacitor dielectrics and composites", PIs: M. Buongiorno Nardelli and J. Bernholc, $140,000, (2010-2013).
- Co-PI: Topological decompositions and spectral sampling algorithms for element substitution in critical technologies, ONR-MURI, (N000141310635) $8,572,268.00; 1 month summer salary (2013-2018).
- Co-PI: Reciprocating Materials Design with the AFLOWLIB.org Repository, ONR, $383,037; 1/2 month summer (2014-2017).
- Co-PI: Mineralogy Genome Project. Extending the aFlow repository to minerals and environmental materials with improved accuracy and fingerprinting, ONR, $300,000; 1/2 month summer (2015-2016).
- Co-PI: NSF-MRI: Acquisition of a Computer Cluster for Computational Modeling at the University North Texas, NSF, $703,000 (2015).
- PI: Clarkson Corporation, AFRL Collaboration Program - Materials and Manufacturing Research, $50,000 (2018)
- Co-PI: DOE - Q4Q: Quantum 1Computation for Quantum Prediction of Materials and Molecular Properties, $465,000 (2018-2022)
- Co-PI: DARPA - HR001121S0026-QB-FP-004, BeQuEST: Benchmarking Quantum Enhancement in Science & Technology, $225,000 (2021-2025)

Current
- Co-PI: DOE-University of Oklahoma, Discovering the mechanism by which polymer porous networks reduce physical aging and plasticization while enhancing permeability and selectivity in microporous polymer membranes, $69,316 (2023-2025)
- Co-PI: DMREF: NSF-NSERC: High Entropy Quantum Materials, $360,389 (total funding $2,000,000.00) (2025-2028)

Activities as External Professor at the Santa Fe Institute

Working groups and workshops

1. December 7-9, 2020 – WG organizer: “Complexity And The Structure Of Music: Universal Features And Evolutionary Perspectives Across Cultures” (co-organized with Miguel Fuentes) – online
2. May 17-20, 2022, WG organizer: “Complexity And Structure Of Music: Universal Features, Evolutionary Processes And Cultural Diversity” (co-organized with Miguel Fuentes)
3. May 30 – June 2, 2023, WG organizer: “Complexity And The Structure Of Music: Universal Features And Evolutionary Perspectives Across Cultures” (co-organized with Miguel Fuentes)
4. June 19-23, 2023, participant: Collective Intelligence Symposium & short course
5. June 10-14, 2024, WG organizer: “Music And Rituals: A Complexity Science Perspective” (co-organized with Edward Slingerland)
6. May 27-29, 2025, WG organizer “Music Evolution from Biology to AI” (co-organized with Elizabeth Margulis and Edward Hagen)

Service as faculty

1. 2021, Santa Fe Institute Complexity Interactive and UCR advisor (Abby Privisova); composer and performance facilitator: “requiem” (online and in studio recording)
2. 2022, CSSS presenter: “Music For Martians”; composer and performance facilitator: “Requiem”
3. 2023, CSSS presenter and workshop facilitator: “Music As Emergence”
4. 2024 –released in March 2025, Complexity Explorer online course design and production: “Music Computation and Complexity”
5. 2025, CSSS instructor: “Music as a Complex Adaptive System”

Outreach

1. May 16, 2022, concert “An Evening Of Music Complexity”, co-sponsored by SFI and Site Santa Fe
2. May 31, 2023, concert of audiovisual works, SFI
3. June 2, 2023, concert with the “Chatter String Quartet”, SFI
4. May 31, 2024, community lecture, SciArt Santa Fe Laser talk “Music For Martians”, Meow Wolf

Media

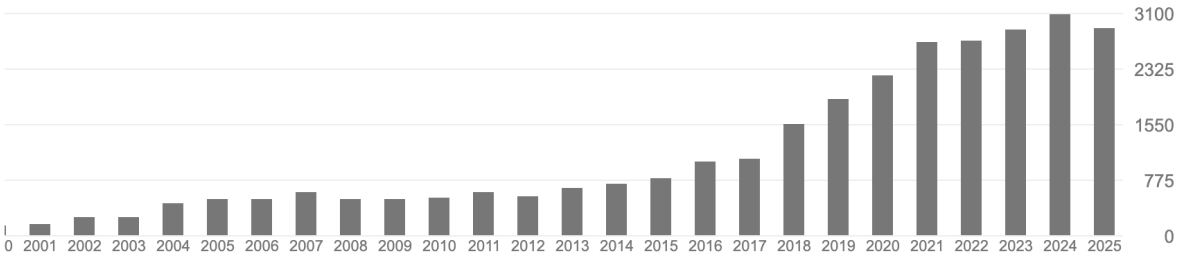
1. September 21, 2022, Miguel Fuentes & Marco Buongiorno Nardelli on Music, Emergence, And Society, Complexity Podcast SFI
2. January 2023, Complexity Explorer journal club: Music Complexity

Publishing

- 2024 – ongoing, special issue on “Music As A Complex Adaptive System”, M. Buongiorno Nardelli, Miguel Fuentes, Tyler Marghetis, Dmitri Tymoczko eds., Advances in Complex Systems (World Scientific)

RESEARCH METRICS

Analysis of the scientific production as of Monday, October 13, 2025



Source: Google Scholar
Sum of the times cited: 30413, (16548 since 2020).
h-index: 68, i-10 index: 159. ResearchGate Research Interest Score: 13,137.
Top 1% in Physics in the Stanford list.
Rank 36 in the Top Italian Scientists in Physics list.

INVITED PAPERS, REVIEW ARTICLES AND BOOKS

1. Kirstin Alberi, Marco Buongiorno Nardelli, Andriy Zakutayev, Lubos Mitas, Stefano Curtarolo, Anubhav Jain, Marco Fornari, Nicola Marzari, Ichiro Takeuchi, Martin L Green, Mercouri G Kanatzidis, Michael F Toney, Sergey Butenko, Bryce Meredig, Stephan Lany, Ursula Kattner, Albert Davydov, Eric Toberer, Vladan Stevanovic, Aron Walsh, Nam-Gyu Park, Alan Aspuru-Guzik, Daniel Tabor, Jenny Nelson, James Murphy, Anant Setlur, John Gregoire, Hong Li, Ruijuan Xiao, Alfred Ludwig, Lane W Martin, Andrew Rappe, Su-Huai Wei, John Perkins, The 2018 Materials by Design Roadmap, Journal of Physics D: Applied Physics (eds. Kirstin Alberi, Marco Buongiorno Nardelli, Andriy Zakutayev) (2018).
2. S. Curtarolo, G. L. W. Hart, M. Buongiorno Nardelli, N. Mingo, S. Sanvito, and O. Levy, The high-throughput highway to computational materials design (invited review), Nature Materials, 12, 191–201 (2013).
3. Erik E. Santiso, Liping Huang, Milen K. Kostov, Aaron M. George, Keith E. Gubbins and Marco Buongiorno Nardelli *Ab initio simulations of chemical reactions in nanostructured carbon materials*, in “Quantum Chemical Calculations of Surfaces and Interfaces of Materials” (Editors: V. A. Basiuk and P. Ugliengo) American Scientific Publishers, (2007).
4. M. Buongiorno Nardelli, V. Meunier and S. Nakhmanson, *Polarization in nanotubes, in “Nanoengineering of structural materials*”, ed. By M. Schulz, A. Kelkar, and M. Sundaresan, CRC Press (Boca Raton, FL, 2005).
5. M. Buongiorno Nardelli and R. McKee, *Un futuro per il nanotransistor (A future for the nanotransistor)*, Le Scienze (Italian edition of “Scientific American”), 422, 70 (2003).

6. J.-L. Fattebert and M. Buongiorno Nardelli, *Finite difference methods for ab initio electronic structure and quantum transport calculations of nanostructures*, in “Handbook of Numerical Analysis”, Volume X, Special volume: Computational Chemistry, edited by C. Le Bris, Elsevier Science, (2003).
7. J. Bernholc, D. Brenner, M. Buongiorno Nardelli, V. Meunier and C. Roland, *Mechanical and electrical properties of nanotubes*, Ann. Rev. Mat. Res. 32, 347 (2002).
8. J. Bernholc, M. Buongiorno Nardelli, J.-L. Fattebert, D. Orlikowski, C. Roland and Q. Zhao, *Mechanical Properties and Electronic Transport in Carbon Nanotubes* , edited by D. Tomanek and R. J. Enbody, Kluwer Academic Publishing, (2000).
9. J. Bernholc, M. Buongiorno Nardelli, D. Orlikowski, C. Roland and Q. Zhao, *Atomic transformations, strength, plasticity and electron transport in strained carbon nanotubes*, in `Fiber Fracture,'' edited by M. Elices, Elsevier, (2000).
10. J. Bernholc, E. L. Briggs, C. Bungaro, M. Buongiorno Nardelli, J.-L. Fattebert, K. Rapcewicz, C. Roland, W. G. Schmidt and Q. Zhao, *Large-Scale Applications of Real-Space Multigrid Methods to Surfaces, Nanotubes, and QuantumTransport*, in `Atomistic Modeling of Materials Properties and Phenomena'' edited by P. Deak, M. Pederson, and T. Frauenheim, Wiley-VCH (1999).
11. S. Baroni, C.M. Bertoni, M. Buongiorno Nardelli, E. Molinari, *Diagonalization of large matrices for large-scale electronic-structure calculations* in `Supercomputing Tools for Science and Engineering'', ed. D. Laforenza and R. Perego, Franco Angeli, Milano, (1990), 645-649.

JOURNAL ARTICLES

1. Karma Tenzin, Berkay Kilic, Raghottam Sattigeri, Zhiren He, Chao Chen Ye, Marcio Costa, Marco Buongiorno Nardelli, Carmine Autieri, Jagoda Slawinska, Persistent spin textures, altermagnetism and charge-to-spin conversion in metallic chiral crystals TM3X6, npj Spintronics, *in press*, (2025).
2. T. T. B. Le, L. Condes, G. D. Barbosa, F. Perez, M. T. Webb, M. Galizia, M. Buongiorno Nardelli and A. Striolo, "Relationship Between Microporous Structure and Light Gases Transport Through Glassy Polymeric Membranes Revealed by Molecular Simulations", J. Mater. Chem. A, 2025, DOI: 10.1039/D5TA02906F
3. Yakandawala, Sasanka A., Gunatilake, Sameera R., Nardelli, Marco Buongiorno, Gunawardena, S. Harshadewa and Liyanage, Laalitha S. I.. "Modelling an amorphous biochar structure using classical molecular dynamics simulations" Pure and Applied Chemistry, 2025. https://doi.org/10.1515/pac-2024-0327
4. Pino D’Amico, Alessandra Catellani, Marco Fornari, Alice Ruini, Marco Buongiorno Nardelli, Stefano Curtarolo, Arrigo Calzolari, Magnetic transparent conductors for spintronic applications, Acta Materialia, 289 (2025) 120850 https://doi.org/10.1016/j.actamat.2025.120850
5. Condes, Lucas; Webb, Matthew; Le, Tran; Box, William; Doherty, Cara; Gali, Aditi; Garrido, Leoncio; Deng, Jing; Matesanz-Niño, Laura; Lozano, Angel E; Alvarez, Cristina; Buongiorno Nardelli, Marco; Striolo, Alberto; Hill, Anita; Galizia, Michele, Elucidating the Molecular Mechanisms by which Porous Polymer Networks Affect Structure, Aging

Propensity, and Selectivity of Microporous Glassy Polymer Membranes using a Multiscale Approach, ACS Applied Materials & Interfaces, 16, 53843 (2024).
6. Karma Tenzin, Arunesh Roy, Homayoun Jafari, Bruno Banas, Frank T. Cerasoli, Mihir Date, Anooja Jayaraj, Marco Buongiorno Nardelli, and Jagoda Sławiǹska, Analogs of Rashba-Edelstein effect from density functional theory, Physical Review B 107, 165140 (2023).
7. Corey Oses, Marco Esters, David Hicks, Simon Divilov, Hagen Eckert, Rico Friedrich, Michael J. Mehl, Andriy Smolyanyuk, Xiomara Campilongo, Axel van de Walle, Jan Schroers, A. Gilad Kusne, Ichiro Takeuchi, Eva Zurek, Marco Buongiorno Nardelli, Marco Fornari, Yoav Lederer, Ohad Levy, Cormac Toher, Stefano Curtarolo, aflow++: A C++ framework for autonomous materials design,
Computational Materials Science, Volume 217, 2023,111889.
8. Jagoda Sławińska, Arunesh Roy, Frank Cerasoli, Anooja Jayaraj, Karma Tenzin, and Marco Buongiorno Nardelli, Long-range current-induced spin accumulation in chiral crystals, npj Computational Materials (2022) 8:243 ; https://doi.org/10.1038/s41524-022-00931-3
9. M. Buongiorno Nardelli, G. Culbreth and M. Fuentes, Evolution of harmonic complexity in western classical music, Advances in Complex
Systems, https://doi.org/10.1142/S0219525922400082 (2022)
10. Quasi-two-dimensional Fermi surface of superconducting line-nodal metal CaSb2, Atsutoshi Ikeda, Shanta Ranjan Saha, David Graf, Prathum Saraf, Danila Sergeevich Sokratov, Yajian Hu, Hidemitsu Takahashi, Soichiro Yamane, Anooja Jayaraj, Jagoda Sławińska, Marco Buongiorno Nardelli, Shingo Yonezawa, Yoshiteru Maeno, and Johnpierre Paglione, Phys. Rev. B 106, 075151.
11. Tuning the electronic and magnetic properties of lizardite clay by chemical substitution MSS Gusmão, A Ghosh, I Siloi, M Fornari, M Buongiorno Nardelli
Molecular Systems Design & Engineering, DOI: 10.1039/D2ME00081D
12. K Sherbert, A Jayaraj, M Buongiorno Nardelli, Quantum algorithm for electronic band structures with local tight-binding orbitals, Scientific reports 12 (1), 1-11
13. Andrew Supka, Nicholas A. Mecholsky, Marco Buongiorno Nardelli, Stefano Curtarolo, Marco Fornari, Two-Layer High-Throughput: Effective Mass Calculations Including Warping,
Engineering, 2022, https://doi.org/10.1016/j.eng.2021.03.031.
14. Anooja Jayaraj, Ilaria Siloi, Marco Fornari & Marco Buongiorno Nardelli, Relaxation time approximations in PAOFLOW 2.0, Scientific Reports volume 12, Article number: 4993 (2022)
15. Kyle Sherbert, Frank Cerasoli and Marco Buongiorno Nardelli, A systematic variational approach to band theory in a quantum computer, RSC Adv., 2021, **11**, 39438-39449
16. Sara Varotto, Luca Nessi, Stefano Cecchi, Jagoda Sławińska, Paul Noel, Simone Petro', Federico Fagiani, Alessandro Novati, Matteo Cantoni, Daniela Petti, Edoardo Albisetti, Marcio Costa, Raffaella Calarco, Marco Buongiorno Nardelli, Manuel Bibes, Silvia Picozzi, Jean-Philippe Attan, Laurent Vila, Riccardo Bertacco and Christian Rinaldi, Room-

temperature ferroelectric switching of spin-to-charge conversion in germanium telluride, Nature Electronics, https://doi.org/10.1038/s41928-021-00653-2 (2021)
17. Marco Buongiorno Nardelli (2021): Tonal harmony and the topology of dynamical score networks, Journal of Mathematics and Music, DOI: https://doi.org/10.1080/17459737.2021.1969599
18. Frank T. Cerasoli, Andrew R. Supka, Anooja Jayaraj, Marcio Costa, Ilaria Siloi, Jagoda Sławińska, Stefano Curtarolo, Marco Fornari, Davide Ceresoli, Marco Buongiorno Nardelli, Advanced modeling of materials with PAOFLOW 2.0: New features and software design, Computational Materials Science, Volume 200, 2021, 110828,
19. DJ Campbell, J Collini, J Sławińska, C Autieri, L Wang, K Wang, B Wilfong, YS Eo, P Neves, D Graf, EE Rodriguez, NP Butch, M Buongiorno Nardelli, J Paglione, Topologically driven linear magnetoresistance in helimagnetic FeP, npj Quantum Materials 6(1), 1-7 (2021).
20. Marcio Costa, Gabriel R Schleder, Carlos Mera Acosta, Antonio CM Padilha, Frank Cerasoli, Marco Buongiorno Nardelli, Adalberto Fazzio, Discovery of higher-order topological insulators using the spin Hall conductivity as a topology signature, npj Computational Materials 7(1), 1-6 (2021).
21. Arrigo Calzolari, Alessandra Catellani, Marco Buongiorno Nardelli, Marco Fornari, Hyperbolic metamaterials with extreme mechanical hardness, Advanced Optical Materials 2001904 (cover article) (2021).
22. Tarik P Cysne, Marcio Costa, Luis M Canonico, M Buongiorno Nardelli, RB Muniz, Tatiana G Rappoport Disentangling orbital and valley Hall effects in bilayers of transition metal dichalcogenides, Physical Review Letters, 126(5), 056601 (2021).
23. Alexander Veremyev, Laalitha Liyanage, Marco Fornari, Vladimir Boginski, Stefano Curtarolo, Sergiy Butenko, Marco Buongiorno Nardelli, Networks of materials: Construction and structural analysis AIChE Journal, 67 (3), e17051 (2021).
24. F. Cerasoli, K.Sherbert, J. Sławińska and M. Buongiorno Nardelli, Quantum computation of silicon electronic band structure Phys. Chem. Chem. Phys., 22 (38), 21816-21822 (2020),
25. Laalitha SI Liyanage, Jagoda Sławińska, Priya Gopal, Stefano Curtarolo, Marco Fornari, Marco Buongiorno Nardelli, High-Throughput Computational Search for Half-Metallic Oxides, Molecules 25 (9), 2010 (2020)
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INVITED TALKS AT CONFERENCES AND WORKSHOPS

1. December 3, 2025, *Computational Frontiers for Quantum Materials*, Zernike Seminar, Zernike Institute for Advanced Materials, University of Groningen, The Netherlands
2. October 6, 2025, *Music for Martians*, colloquium for the series “Mind, Technology and Society (MTS)”, Department of Cognitive Sciences, University of California, Merced
3. September 26, 2025, “Reformulation of DFT+U as a pseudo hybrid Hubbard density functional“, invited talk at "The determination of Hubbard parameters: progress, pitfalls, and prospects" workshop, Gandia (Spain)
4. March 29, 2025, “*Artificial Intelligence and Music: AI tools”*, invited panel for the workshop “Algo-rhythms: the world of Music and AI”, Indiana University Bloomington, IN.
5. March 12, 2025, *“MUSIC” for Martians,* invited colloquium, Department of Physics, Boston College, Boston MA.
6. November 10, 2024 “There is No Time in Music” invited talk at the workshop “*Movement and Time in Art”*, Santa Fe Institute and National Science Foundation, Santa Fe, NM
7. May 31, 2025, *Music for Martians*, SciArt LASER talk, Meow Wolf, Santa Fe, NM
8. April 2-5, 2024, *Network Topology of Generalized Musical Spaces* for the workshop "Space, Scale and Scaling in Art", Isaac Newton Institute*,* Cambridge, UK
9. December 17, 2023, *Networks, topologies and generalized musical spaces*, I Workshop on graph theory and applications, Univ. of Texas, Dallas.
10. November 16, 2023, A network approach to harmonic evolution and complexity in western classical music, CMMR 2023, Tokyo University of Technology, Tokyo, Japan

11. September 7, 2023, 3-4pm CET, *Music as a Complex Adaptive System*, Central European University/Complexity Science Hub joint seminar, Vienna, Austria
12. July 13, 2022, *Network Topology of Generalized Musical Spaces,* IMA Mathematics and Music Conference, London, UK
13. Oct. 21, 2020, : Network Topology of Generalized Musical Spaces: Bach, Euler and the Statistical Mechanics of Music, (virtual) colloquium, Department of Physics, University of Southern California
14. Sept. 22, 2020 Network Topology of Generalized Musical Spaces, NETSCI2020 (virtual)
15. Sept. 17, 2020 Tonal harmony, the topology of dynamical score networks and the Chinese postman problem, NETCENT2020 (virtual)
16. 2019, High-throughput materials discovery and development: breakthroughs and challenges in the mapping of the materials genome, Invited, MRS Fall Meeting 2019.
17. 2018, High-throughput materials discovery and development: breakthroughs and challenges in the mapping of the materials genome, Invited, MRS Fall Meeting 2019.
18. 2018, High-throughput materials discovery and development: breakthroughs and challenges in the mapping of the materials genome, III International Conference on Molecules, Polymers and Material Physics, Manaus (Brazil)
19. 2018, Software engines for fast autonomous screening and characterization of quantum materials, Colloquium, University of Maryland
20. 2017, Novel high-throughput-enabling tools for autonomous screening and characterization of materials. Invited, MRS Fall meeting.
21. 2017, High-throughput discovery and development: software engines for fast autonomous screening and characterization of materials, NGC17, Tomsk (Russia).
22. 2017, High-throughput materials discovery and development: breakthroughs and challenges in the mapping of the materials genome. Invited, MS&T meeting.
23. 2017, High-throughput materials discovery and development: breakthroughs and challenges in the mapping of the materials genome. Invited, APS March Meeting
24. 2016, International Union of Materials Research Societies (IUMRS) International Conference on Electronic Materials (ICEM2016), Singapore, July 4-8.
25. 2016, Symposium MD1 tutorial "Creating the Materials Innovation Infrastructure for Materials by Design", MRS Spring Meeting, March 28-31.
26. 2016, CECAM-INNI workshop "High Throughput materials discovery: perspectives and challenges in theory and experiment" – Tel Aviv, Feb. 3-5.
27. 2016, Advanced Quantum Espresso Developers Meeting: Linear Response, Trieste, Jan. 18-23.
28. 2015, High-throughput materials discovery and development: breakthroughs and challenges in the mapping of the materials genome. Invited, AFRL Forth Walton, FL.
29. 2015, High-throughput materials discovery and development: breakthroughs and challenges in the mapping of the materials genome. Invited, APS March Meeting
30. 2015, High-throughput materials discovery and development: breakthroughs and challenges in the mapping of the materials genome. Invited, Brazilian Physical Society Meeting, Foz de Iguazu - Brazil.

31. 2015, Advanced techniques in materials simulation, Lecturer, University of Sao Paulo - Brazil
32. 2015, High-throughput materials discovery and development: breakthroughs and challenges in the mapping of the materials genome. Keynote speaker, CNMS-ORNL Annual Meeting.
33. 2015, materialssoundmusic, Invited, iARTA- UNT
34. 2015, High-throughput materials discovery and development: breakthroughs and challenges in the mapping of the materials genome. Invited, IMRC – MRS, Cancun, Mexico.
35. 2015, materialssoundmusic: a computer-aided data-driven composition environment for the sonification and dramatization of scientific data streams, Invited, International Computer Music Conference, Denton, TX.
36. 2015, High-throughput materials discovery and development: breakthroughs and challenges in the mapping of the materials genome. Keynote speaker, Metal Oxides Materials Discovery & Applications – Gerusalem, Israel
37. 2015, materialssoundmusic, Colloquium speaker, Music Now series- UNT
38. 2014, Novel tools for accelerated materials discovery: minimal basis projections and the reformulation of DFT+U as a pseudo-hybrid Hubbard density functional. Invited, CSIRO – Cairns, Australia.
39. 2014, High throughput materials discovery and development: using your own computer to search for novel materials (with a little help from the aflowlib.org consortium online library). Invited, MGI workshop – GATech.
40. 2014, High-throughput materials discovery and development: breakthroughs and challenges in the mapping of the materials genome., Invited, ICMEg – Germany.
41. 2014, An introduction to Materials Simulations, Lecturer, Symposium WW – MRS Spring Meeting.
42. 2014, Quantum Espresso workshop. Lecturer, Penn State University.
43. 2013, High-throughput materials discovery and development: breakthroughs and challenges in the mapping of the materials genome, Invited, Computational Sciences and Engineering Conference
44. 2013, Recent advances in first principles theory for high-throughput materials discovery and development, Invited, Materials Research Society, Fall Meeting
45. 2013, Recent advances in molecular transport from first principles, Invited, International Topical Meeting on Nanostructured Materials and Nanotechnology, Morelia, Mexico
46. 2013, High-throughput materials discovery and development: breakthroughs and challenges in the mapping of the materials genome, Speaker, CNMS-ORNL
47. 2013, Recent advances in molecular transport from first principles, Colloquium speaker, University of Arkansas
48. 2013, Computational design of advanced materials for molecular spintronics applications, Invited, American Chemical Society
49. "GPU computing in electronic-structure calculations: accelerating quantum-ESPRESSO and WanT to hybrid architectures", Invited, ORNL, 2012
50. "First Principles Methods and Hydraulic Fracturing: Challenges and Future Perspectives", Invited, NSF, 2012

51. “Quantum-ESPRESSO Summer School”, Lecturer, Penn State University, 2012
52. “Novel paradigms for molecular spintronics: valence tautomeric complexes and graphene functionalizations” Invited, University College, TYC, 2012
53. “Science of Music, Music of Science”, Invited, Imperial College, 2012
54. “First Principles Theory of Charge Mobility and Heat Transport in Graphene-based Systems”. Invited, Imperial College, 2012
55. “First principles design of advanced materials for energy applications”, Invited, “Fundamental Issues at the Interface of Materials and Mechanics Related to Energy Applications” (FIMMEA-2012)
56. “Theory of the electronic and transport properties of epitaxial graphene”, “Specialists Meeting on Carbon”, Puerto Vallarta, Jalisco, Mexico, 26th - 30th September 2011.
57. “Recent advances in molecular electronics and spintronics from first principles”, IV International Conference on Surfaces, Materials and Vacuum", Puerto Vallarta, Jalisco, Mexico, 26th - 30th September 2011.
58. “Recent advances in molecular electronics and spintronics from first principles”, “Materials by Design” workshop, Oak Ridge National Laboratory, Oak Ridge, TN, September 21, 2011.
59. “First principles calculations of charge mobility and heat transport in graphene-based systems”, CNMS Users Meeting, Oak Ridge National Laboratory, Oak Ridge, TN, September 19, 2011.
60. “Electronic and thermal transport in nanostructures”, CECAM workshop on “Thermal and electronic transport”, Lugano (Switzerland) from June 20th to 22nd, 2011.
61. “Theory of the electronic and transport properties of epitaxial graphene”, APS March Meeting 2011.
62. “Recent advances in molecular spintronics from first principles”, XIX International Materials Research Congress, Cancún, México, August 14-18, 2010
63. “First principles calculations of charge mobility and heat transport: a practical tool-set for the efficient design of novel materials and devices for nanoelectronic applications”, XVIII International Materials Research Congress, Cancún, México, August 18-22, 2009
64. “Carbon Nanostructures for Energy and Environmental Applications”, 14th Canadian Semiconductor Technology Conference, Hamilton, Ontario, Canada, August 10-14, 2009.
65. “Polarization Effects and Phase Equilibria in High Energy Density PVDF-Based Polymers”, CECAM workshop on “Structural Transitions in Solids: Theory, Simulations, Experiments and Visualization Techniques”, Lugano, Switzerland, July 8-11, 2009
66. “Carbon Nanostructures for Energy and Environmental Applications”, CECAM workshop on “Modeling of Carbon and Inorganic Nanotubes and Nanostructures”, Lusanne, Switzerland, May 13-15, 2009.
67. “Carbon Nanostructures for Energy and Environmental Applications”, XVII International Materials Research Congress, Cancún, México, August 17-21, 2008
68. "Geometrical phases and the Coulomb buffer in nanoscale interfaces", XVI International Materials Research Congress, Cancún, México, August 19-24, 2007

69. "Wannier Functions and Quantum Transport in Nanostructures", CECAM-psi_k workshop "Maximally Localized Wannier Functions: Concepts, Applications, and Beyond", 27-29 June, 2007, Lyon, France.
70. "Novel advances in the Physics and Chemistry of Carbon Nanotubes", CECAM-psi_k workshop "Simulations of Novel Carbon Materials", 25-28 October 2006, Lyon, France
71. "Electronic transport in nanostructures from first principles", XV International Materials Research Congress, Cancún, México, August 20-24, 2006
72. "Novel advances in the Physics and Chemistry of Carbon Nanotubes", Workshop on "Electronic Structure Methods and their Applications, 10-22 July 2006, Bangalore, India
73. "Iterative solutions of the electronic structure problem", Workshop on "Electronic Structure Methods and their Applications, 10-22 July 2006, Bangalore, India
74. "Interface phases and the Schottky-Mott theory revisited ", 33rd Conference on the Physics and Chemistry of Semiconductor Interfaces (PCSI-33), January 15-19, 2006, in Cocoa Beach, FL.
75. "Interface phases and the Schottky-Mott theory revisited ", ITAMIT Workshop on Computational Materials and Electronics, Austin Texas, October 20-22, 2005.
76. "Crystalline Oxides on Silicon: a future for the nanotransistor", March Meeting of the APS, Los Angeles, CA, March 2005.
77. "The interface phase and the Schottky barrier at a crystalline dielectric on Silicon", IUVSTA 2004, Venice, June 2004.
78. "The interface phase and the Schottky barrier at a crystalline dielectric on Silicon", 5th MOTOROLA workshop on Computational Materials and Electronics, Austin, TX, November 13-14, 2003.
79. "Crystalline Oxides on Semiconductors: a future for the nanotransistor", SESAPS meeting, Wilmington, NC, November 8-10, 2003.
80. "The interface phase and the Schottky barrier for a crystalline dielectric on Silicon",, International Conference on Advanced Materials (IUMRS-ICAM2003), Yokohama, Japan, October 8-10, 2003.
81. `` Quantum transport in nanotube-based structures'', Workshop on "Quantum Phases at the Nanoscale", Centro Ettore Majorana, Erice, Italy, July 15-20, 2002.
82. `` Polarization effects in nanotube structures'', 5th International School on the Applications of Surface Science Techniques, Centro Ettore Majorana, Erice, Italy, July 15-20, 2002.
83. ``Ab initio quantum transport calculations: application to nanostructures'', INFM annual meeting 2002, Bari, Italy, June 24-28, 2002.
84. ``Polarization effects in nanotubolar structures'', Electronic Structure workshop, Berkeley, CA, June 6-8, 2002.
85. ``Quantum transport in nanotube-based structures'', MRS fall meeting, Boston, November 26-30, 2001.
86. ``Electronic and transport properties of carbon nanostructures'', Towards Molecular Electronics, TME'01, Šrem, Poland, June 25-30, 2001.
87. "Quantum Transport in Nanotube-Based Structures", Mardi Gras Conference on Multiscale Simulation, Theoretical, and Experimental Approaches to Deformation, Friction, Fatigue, and Fracture, Baton Rouge, Louisiana, February 2001.

88. ``Electronic and transport properties of carbon nanotubes'', Psi-k Conference, Schwabisch Gmund, Germany, August 22-26, 2000.
89. ``Mechanical deformations and electronic transport in carbon nanotubes'', MRS Spring Meeting, San Francisco, April 24-28, 2000.
90. ``Theory of electronic and transport properties of carbon nanotubes'', APS March Meeting, Minneapolis, Indiana, March 2000.
91. ``Mechanical and transport properties of carbon nanotubes'', ``Fullerenes 99'' workshop, Aug. 29-Sep. 2, 1999, Chateau de Bonas, France.
92. ``Electronic transport in nanostructures: application to carbon nanotubes'', workshop on ``New methods in electronic structure'', May 21-24, 1999, Urbana, IL.
93. ``Brittle and ductile behaviour in carbon nanotubes'', 9th ``International Workshop on Computational Materials Science: Electronic Structure Theory and Simulations'', 14-16 January 1999, Trieste, Italy.
94. ``Growth and mechanical properties of Carbon Nanotubes'', MRS Fall Meeting, Boston, November 30-December 4, 1998.
95. ``Wide-gap nitrides: from growth morphology to device behavior'', M. Buongiorno Nardelli, K. Rapcewicz, C. Bungaro, E.L. Briggs and J. Bernholc, APS March Meeting, Los Angeles, California, March 1998.
96. ``Theory of Surfaces, Adsorbates, Heterostructures, Defects and Ordering in Nitride Semiconductors'', J. Bernholc, P. Boguslawski, C. Bungaro, M. Buongiorno Nardelli and K. Rapcewicz, International GaN Workshop at Schloss Ringberg, ``Surface Morphology, Interfaces and Growth of the III-Nitrides'', Schloss Ringberg, Germany, January 20 - 24 1998.
97. ``Theory of Surfaces and Interfaces in Wide-Gap Nitrides.'' M. Buongiorno Nardelli, K. Rapcewicz and J. Bernholc, Electronic Structure 1997 Workshop, Cornell University, Ithaca, New York, May 1997.
98. ``Theory of Growth and Mechanical Properties of Carbon Nanotubes.'' J. Bernholc, C. J. Brabec, M. Buongiorno Nardelli, M.-P. Campbell, A. Maiti, K. Rapcewicz, C. Roland, and B. I. Yakobson, Carbon Nanotube Workshop, Rice University, Houston, Texas, May 1997.
99. ``Theory of Surfaces and Interfaces in Wide-Gap Nitrides.'' K. Rapcewicz, M. Buongiorno Nardelli and J. Bernholc, APS March Meeting, Kansas City, Missouri, March 1997.
100. ``Real-Space Multigrid Calculations for Surfaces, Interfaces, and Proteins.'' J. Bernholc, C. Brabec, E.L. Briggs, M. Buongiorno Nardelli, K. Rapcewicz, C. Roland, M. Wensell, APS March Meeting, Kansas City, Missouri, March 1997.
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