

Personal data

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Education

- 2004 **Ph.D. in Physics**, Ecole Polytechnique Fédérale de Lausanne (EPFL, Switzerland).
Thesis: *First-principles molecular-dynamics study of metal-supported nanosystems*.
Advisor: Prof. A. Baldereschi.
- 1999 **“Laurea” (Diploma) in Physics** 110/110 cum laude, University of Trieste (Italy).

Research Employment

- 2011- **ICREA Research Professor**, Institut de Ciència de Materials de Barcelona (ICMAB-CSIC).
- 2010-11 **“Ramón y Cajal” fellow (PI)**, ICMAB-CSIC.
- 2009 **Postdoctoral researcher**, CECAM-EPFL, Switzerland (W. Andreoni group)
- 2005-2009 **Postdoctoral Researcher**, University of California, Santa Barbara, USA (N. Spaldin group)
- 2005 **Postdoctoral Researcher**, EPFL, Switzerland (A. Baldereschi group)

Grants/awards as principal investigator

- 2024-27 **MICiU Grant**. *Linear response of INSulators with broken SPace-Inversion or time-REversal symmetries from first principles (INSPIRE)*.
Budget: 80,000 € + 1 FPI fellowship
- 2017-23 **ERC Consolidator Grant**. *Hierarchical multiscale modeling of flexoelectricity and related materials properties from first principles (MULTIFLEXO)*.
Budget: 1,470,000 €
- 2020-23 **MINECO Grant** (proyectos I+D+i). *Functional Oxide Single-crystal Membranes (FOxMe)*
Budget: 84,700 €
- 2016-19 **MINECO Grant** (proyectos I+D+i excelencia). *Phase and Antiphase Boundaries and Domains in Antiferroelectrics (PHABADA)*.
Budget: 50,000 €
- 2014-17 **MINECO Grant** (proyectos I+D+i excelencia). *Oxide stresstronics (OSTRES)*.
Budget: 22,000 € + 1 FPI fellowship
- 2009-11 **“Ramón y Cajal” fellowship**

Committees and associations

Member of the International Advisory Committee of ABINIT since June 2021.
Active member of the American Physical Society (APS).

Teaching Experience

- 2002-04 Assistant to undergraduate courses: Physics I (Prof. H. Brune) and Numerical Simulation (Prof. A. Baldereschi), EPFL, Switzerland.
- 2006-09 Research supervisor to junior graduate student researcher (J. M. Rondinelli), UCSB, USA.

PhD theses

- 2019-24 Asier Zabalo Alonso. "*First-principles theory of spatial dispersion.*" Defense: November 8th, 2024.
- 2018-24 Matteo Springolo. "*Flexoelectricity in two-dimensional materials from density-functional perturbation theory.*" Defense: April 9th, 2024.
- 2014-19 Andrea Maria Enrico Schiaffino. "*First-principles theory of flexoelectricity: methods and applications.*" Defense: July 2nd, 2019.

Master theses

- 2019 Asier Zabalo Alonso. "*Switching a polar metal via strain gradients.*" Defense: July 21th, 2019.

Research stays

- 2-6/2024 Sabbatical leave at the Center for Computational Quantum physics, Flatiron Institute, New York.

Other merits

- Referee for Nature, Nature Materials, Physical Review Letters, Physical Review X, Physical Review B, Scientific Reports, Nature Communications, Journal of Physics: Condensed Matter, Europhysics Letters, Advanced Functional Materials, Applied Physics Letters, Nature Physics.
- External grant reviewer for the US National Science Foundation and ERC.
- Co-organizer with J. Íñiguez (ICMAB-CSIC) of a CECAM workshop (<http://www.cecarn.org/workshop-469.html>) on "*Theory of Magnetoelectrics*", held in Lausanne (Switzerland) on May 26-28, 2010.
- Co-organizer with J. Íñiguez, P. Ordejón and D. Sanchez-Portal of the "*Mini-2012*" conference (<http://www.cecarn.org/workshop-621.html>), held in Barcelona, January 12-14, 2012.
- Co-organizer with V. Gopalan and S.-W. Cheong of a Focus Session on Dielectric and Ferroic Oxides at the APS March Meeting 2015 in San Antonio, TX.
- Session chair at APS March Meeting 2008 in New Orleans, LA; "Total Energy" workshop 2011 in Trieste (Italy); MRS Spring Meeting 2013 in San Francisco, CA; MRS Fall Meeting 2014 in Boston, MA.

Research summary

- 11 invited talks at international conferences since 2020
- 28 publications since 2020, including 12 Phys. Rev. Lett. and 4 Phys. Rev. X
- 3 PhD theses finalized in total, 2 since 2020
- h-index = 38 (Web of Science), 43 (Google Scholar).

Research group

- Miquel Royo. Staff scientist at ICMAB since October 2021 (formerly postdoc 2017-21).
- Asier Zabalo Alonso. Postdoc since November 2024 (formerly PhD student 2018-24).
- Guglielmo Marchese. Postdoc since November 2024.

Former members

- Matteo Springolo. Ph.D. student, March 2018 to April 2024.
- Konstantin Shapovalov. Postdoc, March 2018 to June 2023.
- Alexander Edström. Postdoc (grant of the Swedish Research Council), November 2019 to October 2022.
- Madhura Marathe. Postdoc (Marie Curie COFUND), July 2017 to June 2020.
- Andrea Maria Enrico Schiaffino. Ph.D. student, January 2015 to July 2019.
- Konstanze R. Hahn. Postdoc, November 2017 to June 2019.
- Claudio Cazorla. Postdoc (JAE-Doc fellowship), December 2010 to July 2014.

Peer-reviewed journal articles

2024

- [82] Michele Conroy, Didrik René Småbråten, Colin Ophus, Konstantin Shapovalov, Quentin M Ramasse, Kasper Aas Hunnestad, Sverre M Selbach, Ulrich Aschauer, Kalani Moore, J Marty Gregg, Ursel Bangert, Massimiliano Stengel, Alexei Gruverman, Dennis Meier, *Observation of antiferroelectric domain walls in a uniaxial hyperferroelectric*, **Advanced Materials** 36 (39), 2405150
- [81] I Souza, RM Martin, M Stengel, *Optical bounds on many-electron localization*, arXiv preprint arXiv:2407.17908.
- [80] A Zabalo, M Stengel, *Ensemble density functional perturbation theory: Spatial dispersion in metals*, **Physical Review B** 109 (24), 245116
- [79] M. Stengel, *Macroscopic polarization from nonlinear gradient couplings*, **Physical Review Letters** 132 (14), 146801
- [78] Shang Ren, John Bonini, Massimiliano Stengel, Cyrus E. Dreyer, David Vanderbilt, *Adiabatic dynamics of coupled spins and phonons in magnetic insulators*, **Phys. Rev. X** 14 (1), 011041.

2023

- [77] Matteo Springolo, Miquel Royo, and Massimiliano Stengel, *In-Plane Flexoelectricity in Two-Dimensional D_{3d} Crystals*, **Phys. Rev. Lett.** 131, 236203 (2023)
- [76] Asier Zabalo and Massimiliano Stengel, *Natural Optical Activity from Density-Functional Perturbation Theory*, **Phys. Rev. Lett.** 131, 086902 (2023)
- [75] K Shapovalov and M Stengel, *Tilt-driven antiferroelectricity in $PbZrO_3$* , **Physical Review Materials** 7 (7), L071401.
- [74] C Cazorla, M Stengel, J Íñiguez, R Rurali, *Giant multiphononic effect in a perovskite oxide*, **npj Computational Materials** 9 (1), 97.
- [73] S. Ponce, M Royo, M Stengel, N Marzari, M Gibertini, *Long-range electrostatic contribution to electron-phonon couplings and mobilities of two-dimensional and bulk materials*, **Physical Review B** 107 (15), 155424.
- [72] Samuel Poncé, Miquel Royo, Marco Gibertini, Nicola Marzari, and Massimiliano Stengel, *Accurate Prediction of Hall Mobilities in Two-Dimensional Materials through Gauge-Covariant Quadrupolar Contributions*, **Phys. Rev. Lett.** 130, 166301 (2023)
- [71] Bonini, J.; Ren, S; Vanderbilt, D.; Stengel, M.; Dreyer, C. E.; Coh, S., *'Frequency splitting of chiral phonons from broken time.reversal symmetry in CrI_3 '*, **Physical Review Letters**, 130, 086701 (2023)

2022

- [70] Diéguez, Oswaldo and Stengel, Massimiliano, *'Translational covariance of flexoelectricity at ferroelectric domain walls'*, **Physical Review X**, 12, 031002.

- [69] Edström, A; Amoroso, D; Picozzi, S.; Barone, P.; Stengel, M., '*Curved magnetism in CrI3*', **Physical Review Letters**, 128, 177202. (**Editors' Suggestion.**)
- [68] Dreyer, CE; Coh, S; Stengel, M, '*Nonadiabatic Born Effective Charges in Metals and the Drude Weight*', **Physical Review Letters**, 128, 095901. (**Editors' Suggestion.**)
- [67] H Wang, F Tang, M Stengel, H Xiang, Q An, T Low, X Wu, '*Convert widespread paraelectric perovskite to ferroelectrics*', **Physical Review Letters** 128 (19), 197601
- [66] Zabalo, A; Dreyer, CE; Stengel, M, '*Rotational g factors and Lorentz forces of molecules and solids from density functional perturbation theory*', **Physical Review B**, 105, 094305.
- [65] Royo, Miquel; Stengel, Massimiliano, '*Lattice-mediated bulk flexoelectricity from first principles*', **Physical Review B**, 105, 064101.

2021

- [64] Aramberri, H; Cazorla, C; Stengel, M; Iniguez, J, '*On the possibility that PbZrO3 not be antiferroelectric*', **NPJ Computational Materials**, 7, 196.
- [63] Springolo, Matteo; Royo, Miquel; Stengel, Massimiliano, '*Direct and converse flexoelectricity in two-dimensional materials*', **Physical Review Letters**, 127, 216801.
- [62] Royo, Miquel; Stengel, Massimiliano, '*Exact long-range dielectric screening and interatomic forces in quasi-2D crystals*', **Physical Review X**, 11, 041027.
- [61] Zabalo, Asier; Stengel, Massimiliano, '*Switching a polar metal via strain gradients*', **Physical Review Letters**, 126, 127601.

2020

- [60] Royo, Miquel; Hahn, Konstanze R.; Stengel, Massimiliano, '*Using High Multipolar Orders to Reconstruct the Sound Velocity in Piezoelectrics from Lattice Dynamics*', **Physical Review Letters**, 125, 217602.
- [59] Stefani, Christina; Ponet, Louis; Shapovalov, Konstantin; et al., '*Mechanical Softness of Ferroelectric 180 degrees Domain Walls*', **Physical Review X**, 10, 041001.
- [58] Brunin, Guillaume; Coutada Miranda, Henrique Pereira; Giantomassi, Matteo; et al., '*Phonon-limited electron mobility in Si, GaAs, and GaP with exact treatment of dynamical quadrupoles*', **Physical Review B**, 102, 094308.
- [57] Brunin, Guillaume; Coutada Miranda, Henrique Pereira; Giantomassi, Matteo; et al., '*Electron-Phonon beyond Fröhlich: Dynamical Quadrupoles in Polar and Covalent Solids*', **Physical Review Letters**, 125, 136601.
- [56] McGilly, Leo J.; Kerelsky, Alexander; Finney, Nathan R.; et al., '*Visualization of Moiré superlattices*', **Nature Nanotechnology**, 15, 580.
- [55] Shu, Longlong; Ke, Shanming; Fei, Linfeng; ... ; Stengel, Massimiliano; Catalan, Gustau, '*Photoflexoelectric effect in halide perovskites*', **Nature Materials**, 19, 605.

[54] Romero, Aldo H.; Allan, Douglas C.; Amadon, Bernard; et al., '*ABINIT: Overview and focus on selected capabilities*', **Journal of Chemical Physics**, 152, 124102.

2019

[53] Schaab, J.; Shapovalov, K.; Schoenherr, P.; Hackl, J.; Khan, M., I; Hentschel, M.; Yan, Z.; Bourret, E.; Schneider, C. M.; Nemsk, S.; Stengel, M.; Cano, A.; Meier, D., '*Electrostatic potential mapping at ferroelectric domain walls by low-temperature photoemission electron microscopy*', **Applied Physics Letters** 115, 122903.

[52] Menendez, Enric; Sireus, Veronica; Quintana, Alberto; Fina, Ignasi; Casals, Blai; Cichelero, Rafael; Kataja, Mikko; Stengel, Massimiliano; Herranz, Gervasi; Catalan, Gustau; Baro, Maria Dolores; Surinach, Santiago; Sort, Jordi, '*Disentangling Highly Asymmetric Magnetoelectric Effects in Engineered Multiferroic Heterostructures*', **Physical Review Applied** 12, 014041.

[51] Junquera, Javier; Garcia-Fernandez, Pablo; Stengel, Massimiliano, '*Mechanisms to enhance the capacitance beyond the classical limits in capacitors with free-electron-like electrodes*', **Physical Review B**, 99, 235127.

[50] Schiaffino, Andrea; Dreyer, Cyrus E.; Vanderbilt, David; Stengel, Massimiliano, '*Metric wave approach to flexoelectricity within density functional perturbation theory*', **Physical Review B**, 99, 085107. (**Editors' Suggestion.**)

[49] Schoenherr, Peggy; Shapovalov, Konstantin; Schaab, Jakob; Yan, Zewu; Bourret, Edith D.; Hentschel, Mario; Stengel, Massimiliano; Fiebig, Manfred; Cano, Andres; Meier, Dennis 2019, '*Observation of Uncompensated Bound Charges at Improper Ferroelectric Domain Walls*', **Nano Letters**, 19, 1659 - 1664.

[48] Royo, Miguel; Stengel, Massimiliano, '*First-Principles Theory of Spatial Dispersion: Dynamical Quadrupoles and Flexoelectricity*', **Physical Review X**, 9, 021050.

2018

[47] Dreyer, Cyrus E.; Stengel, Massimiliano; Vanderbilt, David, '*Current-density implementation for calculating flexoelectric coefficients*', **Physical Review B** 98, 075153. (**Editors' Suggestion.**)

[46] Casals, Blai; Schiaffino, Andrea; Casiraghi, Arianna; Hamalainen, Sampo J.; Gonzalez, Diego Lopez; van Dijken, Sebastiaan; Stengel, Massimiliano; Herranz, Gervasi, '*Low-Temperature Dielectric Anisotropy Driven by an Antiferroelectric Mode in SrTiO₃*', **Physical Review Letters**, 120, 217601.

[45] Stengel, Massimiliano; Vanderbilt, David, '*Quantum theory of mechanical deformations*', **Physical Review B**, 98, 125133.

2017

[44] Gazquez J, Stengel M, Mishra R, Scigaj M, Varela M, Roldan MA, Fontcuberta J, Sanchez F & Herranz G, '*Competition between Polar and Nonpolar Lattice Distortions in Oxide Quantum Wells: New Critical Thickness at Polar Interfaces*', **Physical Review Letters**, 119, 106102.

[43] Schiaffino A & Stengel M, '*Macroscopic Polarization from Antiferrodistortive Cycloids in Ferroelastic SrTiO₃*', **Physical Review Letters**, 119, 137601.

[42] Mundy JA, Schaab J, Kumagai Y, Cano A, Stengel M, Krug IP, Gottlob DM, Doganay H, Holtz

ME, Held R, Yan Z, Bourret E, Schneider CM, Schlom DG, Muller DA, Ramesh R, Spaldin NA & Meier D, '*Functional electronic inversion layers at ferroelectric domain walls*', **Nature Materials**, 16, 622.

2016

- [41] Stengel M, '*Unified ab initio formulation of flexoelectricity and strain-gradient elasticity*', **Physical Review B**, 93, 245107. (**Editors' Suggestion.**)
- [40] Salje EKH, Li S, Stengel M, Gumbsch P & Ding X, '*Flexoelectricity and the polarity of complex ferroelastic twin patterns*', **Physical Review B**, 94, 024114.

2015

- [39] Cazorla C & Stengel M 2015, '*Electrostatic engineering of strained ferroelectric perovskites from first principles*', **Phys. Rev. B** 92, 214108.
- [38] Stengel M, '*From flexoelectricity to absolute deformation potentials: The case of SrTiO₃*', **Phys. Rev. B** 92, 205115.
- [37] Stengel M & Íñiguez J, '*Electrical phase diagram of bulk BiFeO₃*', **Phys. Rev. B** 92, 235148. (**Editors' Suggestion.**)
- [36] Narváez J, Saremi S, Hong J, Stengel M & Catalan G, '*Large Flexoelectric Anisotropy in Paraelectric Barium Titanate*', **Physical Review Letters** 115, 037601.

2014

- [35] J. Íñiguez, M. Stengel, S. Prosandeev, and L. Bellaiche, '*First-principles study of the multimode antiferroelectric transition in PbZrO₃*', **Phys. Rev. B (Rapid Comm.)** 90, 220103(R) (2014).
- [34] C. Cazorla and M. Stengel, '*Ab initio design of charge-mismatched ferroelectric superlattices*', **Phys. Rev. B (Rapid Comm.)** 90, 020101(R) (2014).
- [33] M. Stengel, '*Surface Control of Flexoelectricity*', **Phys. Rev. B (Rapid Comm.)** 90, 201112(R) (2014).

2013

- [32] M. Stengel, '*Microscopic response to inhomogeneous deformations in curvilinear coordinates*', **Nature Communications** 4, 2693 (2013).
- [31] M. Stengel, '*Flexoelectricity from density-functional perturbation theory*', **Physical Review B** 88, 174106 (2013).
- [30] N. C. Bristowe, M. Stengel, P. B. Littlewood, E. Artacho, J. M. Pruneda, '*One-dimensional half-metallic interfaces of two-dimensional honeycomb insulators*', **Physical Review B** 88, 161411 (2013).

2012

- [29] C. Ocal, R. Bachelet, L. Garzon, M. Stengel, F. Sanchez and J. Fontcuberta, '*Nanoscale*

Laterally Modulated Properties of Oxide Ultrathin Films by Substrate Termination Replica through Layer-by-Layer Growth, **Chemistry of Materials** 24, 4177-4184 (2012).

- [28] Y. Yang, M. Stengel, W. Ren, X. H. Yan and L. Bellaiche, *Epitaxial short-period PbTiO₃/BiFeO₃ superlattices studied by first-principles calculations*, **Physical Review B** 86, 144114 (2012).
- [27] M. Stengel, C. J. Fennie and Ph. Ghosez, *Electrical properties of improper ferroelectrics from first principles*, **Physical Review B** 86, 094112 (2012). (**Editors' Suggestion.**)
- [26] Y. Yang, W. Ren, M. Stengel, X. H. Yan and L. Bellaiche, *Revisiting Properties of Ferroelectric and Multiferroic Thin Films under Tensile Strain from First Principles*, **Physical Review Letters** 109, 057602 (2012).
- [25] C. Cazorla and M. Stengel, *First-principles modeling of Pt/LaAlO₃/SrTiO₃ capacitors under an external bias potential*, **Physical Review B** 85, 075426 (2012).
- [24] N. C. Bristowe, M. Stengel, P. B. Littlewood, J. M. Pruneda, E. Artacho, *Electrochemical ferroelectric switching: Origin of polarization reversal in thin films*, **Physical Review B** 85, 024106 (2012).

2000-2011

- [23] M. Stengel, *Electrostatic stability of insulating surfaces: Theory and applications*, **Phys. Rev. B** 84, 205432 (2011).
- [22] C. Cancellieri, D. Fontaine, S. Gariglio, N. Reyren, A. D. Caviglia, A. Fete, S. J. Leake, S. A. Pauli, P. R. Willmott, M. Stengel, Ph. Ghosez, and J.-M. Triscone, *Electrostriction at the LaAlO₃/SrTiO₃ interface*, **Physical Review Letters** 107, 056102 (2011).
- [21] M. Stengel, *First-principles modeling of electrostatically doped perovskite systems*, **Phys. Rev. Lett.** 106, 136803 (2011).
- [20] M. Stengel, P. Aguado-Puente, N. A. Spaldin and J. Junquera, *Band alignment at metal/ferroelectric interfaces: Insights and artifacts from first principles*, **Physical Review B** 83, 235112 (2011). (**Editors' Suggestion.**)
- [19] G. Tomba, M. Stengel, W.-D. Schneider, A. Baldereschi, and A. De Vita, *Supramolecular Self-Assembly Driven by Electrostatic Repulsion: . . .*, **ACS Nano** 4, 7545 (2010).
- [18] A. Roy, M. Stengel and D. Vanderbilt, *First-principles study of high-field piezoelectricity in tetragonal PbTiO₃*, **Physical Review B** 81, 014102 (2010).
- [17] M. Stengel, D. Vanderbilt and N. A. Spaldin, *First-principles modeling of ferroelectric capacitors via constrained-D calculations*, **Physical Review B** 80, 224110 (2009). (**Editors' Suggestion.**)
- [16] M. Stengel and D. Vanderbilt, *Berry-phase theory of polar discontinuities at oxide-oxide interfaces*, **Physical Review B (Rapid Comm.)** 80, 241103(R) (2009). (**Editors' Suggestion.**)

- [15] M. Stengel, D. Vanderbilt and N. A. Spaldin, *Enhancement of ferroelectricity at metal/oxide interfaces*, **Nature Materials** 8, 392 (2009).
- [14] M. Stengel, N. A. Spaldin and D. Vanderbilt, *Electric displacement as the fundamental variable in electronic-structure calculations*, **Nature Physics** 5, 304 (2009).
- [13] J. M. Rondinelli, M. Stengel and N. A. Spaldin, *Carrier-mediated magnetoelectricity in complex oxide heterostructures*, **Nature Nanotechnology** 3, 46 (2008).
- [12] X. Wu, M. Stengel, K. M. Rabe, D. Vanderbilt, *Predicting polarization and nonlinear dielectric response of superlattices*, **Phys. Rev. Lett.** 101, 087601 (2008). (**Editors' Suggestion.**)
- [11] M. Stengel and N. A. Spaldin, *Self-interaction correction with Wannier functions*, **Phys. Rev. B** 77, 155106 (2008).
- [10] M. Stengel and N. A. Spaldin, *Ab-initio theory of metal-insulator interfaces in a finite electric field*, **Phys. Rev. B** 75, 205121 (2007).
- [9] M. Stengel and N. A. Spaldin, *Origin of the dielectric dead layer in nanoscale capacitors*, **Nature** 443, 679 (2006).
- [8] M. Stengel and N. A. Spaldin, *Accurate polarization within a unified Wannier function formalism*, **Phys. Rev. B** 73, 075121 (2006).
- [7] M. Pivetta, F. Patthey, M. Stengel, A. Baldereschi, and W.-D. Schneider, *Local work function Moiré pattern on ultrathin ionic films: . . .*, **Phys. Rev. B** 72, 115404 (2005).
- [6] S. Schintke, M. Stengel, . . . , and A. De Vita, Euro Ceramics VIII, Pts. 1-3 Key Engineering Materials 264-268, 485-488 (2004).
- [5] M. Stengel, A. De Vita and A. Baldereschi, *Adatom-Vacancy Mechanisms for the C60/Al(111) (6 × 6) Reconstruction*, **Phys. Rev. Lett.** 91, 166101 (2003).
- [4] R. Gruber, P. Volgers, A. De Vita, M. Stengel and T.-M. Tran, *Parameterisation to tailor commodity clusters to applications*, **Fut. Gen. Comp. Sys.** 19, 111 (2003).
- [3] M. Vladimirova, M. Stengel, A. De Vita, A. Baldereschi, M. Bohringer, K. Morgenstern, R. Berndt and W.-D. Schneider, *Supramolecular self-assembly and selective step decoration on the Au(111) surface*, **Europhys. Lett.** 56, 254 (2001).
- [2] S. Schintke, S. Messerli, M. Pivetta, F. Patthey, L. Libioulle, M. Stengel, A. De Vita and W. D. Schneider, *Insulator at the Ultrathin Limit: MgO on Ag(001)*, **Phys. Rev. Lett.** 87, 276801 (2001).
- [1] M. Stengel and A. De Vita, *First-principles molecular dynamics of metals: A Lagrangian formulation*, **Phys. Rev. B** 62, 15283 (2000).

Other publications

[1] N. A. Benedek and M. Stengel, *Viewpoint: Polarization that holds steady*, **Physics** 7, 32 (2014).

Book chapters

[B1] C. Lichtensteiger, P. Zubko, M. Stengel, P. Aguado-Puente, J.-M. Triscone, Ph. Ghosez and J. Junquera, "*Ferroelectricity in ultrathin film capacitors*". In G. Pacchioni and S. Valeri, editors. "Oxide ultrathin films: science and technology". J. Wiley & Sons, 2011.

[B2] Stengel M & Vanderbilt D, "*First-principles theory of flexoelectricity*", in *Flexoelectricity in Solids: From Theory to Applications*, Tagantsev AK & Yudin P, eds. (World Scientific, Singapore, 2016).

Invited talks at international conferences and workshops.

- [50] *Lattice dynamics in systems with broken time-reversal symmetry*. Total Energy and Force Methods Conference (Trieste, January 8-10, 2025).
- [49] *Macroscopic polarization from nonlinear gradient couplings*. Fundamental Physics of Ferroelectrics and related materials workshop (Washington DC, February 4-7, 2024).
- [48] *Flexomagnetism and chiral phonons in CrI₃*. Magnons and Magnetism in 2D Materials (Valencia, October 18-19, 2023)
- [47] *Flexoelectricity and flexomagnetism in two-dimensional materials*. CMD30 FisMat2023 joint conference (Politecnico di Milano, September 2023).
- [46] *Flexoelectricity and long-range Coulomb interactions in two-dimensional crystals*. CMT@Brixen Workshop (Bressanone/Brixen, June 2023).
- [45] *Flexoelectricity and long-range Coulomb interactions: from 3D to 2D*. 5th Anniversary Conference of CCQ (NYC, June 2022).
- [44] *Flexoelectricity and long-range Coulomb interactions: from 3D to 2D*. 2022 Workshop on Recent Developments in Electronic Structure (ES22), Columbia University (NYC, June 2022).
- [43] *Long-range dielectric screening and force constants in two dimensions*. ABINIT developer workshop (online, June 2021)
- [42] *Long-range dielectric screening and force constants in two dimensions*. Total Energy Workshop (online, February 2021)
- [41] *The bulk flexoelectric tensor from an ab initio perspective*. Fundamental physics of Ferroelectrics Workshop (online, January 2021).
- [40] *First-principles theory of flexoelectricity and related materials properties*. Workshop on Total Energy and Force Methods, San Sebastian-Donostia (January 2000).
- [39] *New functionalities from gradients: Flexoelectricity and more*. European Meeting on Ferroelectricity (EMF), Lausanne (July 2019)
- [38] *New functionalities from gradients: Flexoelectricity and more*. International Workshop on Topological Structures in Ferroic Materials - TOPO2019, Prague (Czech Republic).
- [37] *Lautrec*. Alessandro De Vita: A Celebration of his Life and Work. King's College (London), May 2019.
- [36] *First-principles theory of spatial dispersion effects*. ABINIT developer workshop, Louvain-la-Neuve, May 2019.
- [35] *Macroscopic polarization from antiferrodistortive cycloids in ferroelastic SrTiO₃*. Korea Advanced Institute of Science and Technology (KAIST). November 2018.
- [34] *Macroscopic polarization from antiferrodistortive cycloids in ferroelastic SrTiO₃*. 14th International Symposium on Ferroic Domains (ISFD), Barcelona (Spain). September 2018.
- [33] *Macroscopic polarization from antiferrodistortive cycloids in ferroelastic SrTiO₃*. International Workshop on Topological Structures in Ferroic Materials - TOPO2018, Natal (Brazil).
- [32] *New functionalities from gradients: Flexoelectricity and more*. APS March Meeting, Los Angeles, CA (Mar, 2018)
- [31] *Macroscopic polarization from antiferrodistortive cycloids in ferroelastic SrTiO₃*. CECAM Workshop on Ferroelectric Domain Walls, Tel Aviv University, November 2017.
- [30] *First-principles theory of flexoelectricity*. 27th annual Workshop on the Fundamental Physics of Ferroelectrics. Washington, DC (January 2016).

- [29] *Flexoelectricity via coordinate transformations*. E-MRS Fall Meeting, Warsaw, Poland (9/2015).
- [28] *Flexoelectricity from density-functional perturbation theory*. Ψ -k Conference, San Sebastian, Spain (9/2015).
- [27] *Flexoelectricity via coordinate transformations*. European Meeting on Ferroelectricity, Porto, Portugal (6/2015).
- [26] *Surface Control of Flexoelectricity*. International Workshop on Relaxor Ferroelectrics, Stirin, Czech Republic (October 2014).
- [25] *Surface Control of Flexoelectricity*. E-MRS Fall Meeting, Warsaw, Poland (September 2014).
- [24] *Flexoelectricity via coordinate transformations*. Workshop on Complex Oxides, Protaras, Cyprus (July 2014).
- [23] *Flexoelectricity via coordinate transformations*. APS March Meeting, Denver, CO (March 2014).
- [22] *Flexoelectricity via coordinate transformations*. Challenges in Multiferroics/Magnetolectrics Workshop, Strasbourg, France (December 2013).
- [21] *Polar Discontinuities and Compensation Mechanisms at Oxide-oxide Interfaces*. MRS Meeting, San Francisco, CA (2013).
- [20] *Macroscopic electrostatics at the nanoscale: From ferroelectric capacitors to confined electron gases*. APS March Meeting, Boston, MA (2012).
- [19] *First-principles nanoelectronics: Oxide thin-film devices by design*. GEFES 2012 - VII Reunión del Grupo Especializado de Física de Estado Sólido. Sevilla, Andalucía, España (2012).
- [18] *Macroscopic Electrostatics and Chemical Bonding in Ferroelectric Nanocapacitors*. European Meeting on Ferroelectricity, Bordeaux (June 2011).
- [17] *Macroscopic electrostatics at oxide-oxide interfaces: From ferroelectric capacitors to confined electron gases*. Workshop on Advanced Oxide Interfaces, ICTP Trieste, Italy (May 2011).
- [16] *First-principles nanoelectronics: Oxide thin-film devices by design*. ψ k Conference 2010, September 2010, Berlin (Germany).
- [15] *Electrostatics and chemical bonding at metal-oxide interfaces*. CECAM Workshop on Ab-initio electrochemistry, July 2010, Lausanne (Switzerland).
- [14] *"Proper" treatment of the macroscopic variables in multiferroic systems*. CECAM Workshop on Theory of Multiferroics, May 2010, Lausanne (Switzerland).
- [13] *"Proper" treatment of the macroscopic variables in multiferroic systems*. Workshop on Computational Magnetism and Spintronics, May 2010, Bonn (Germany).
- [12] *First-principles nanoelectronics: Oxide thin-film devices by design*. Workshop on Fundamental Physics of Ferroelectrics 2010, Aspen, CO.
- [11] *First-principles nanoelectronics: Oxide thin-film devices by design*. Mini-2010 conference, January 2010, Shanghai, China.
- [10] *First-principles nanoelectronics: Oxide thin-film devices by design*. Electronic Structure Conference 2009, UC Davis, Davis, CA.
- [9] *Dielectric, Piezoelectric and Magnetolectric Properties via First-Principles Calculations at Constant Electric Displacement*. MRS Spring Meeting 2009, San Francisco, CA.
- [8] *Electrostatics of metal-oxide interfaces from first principles*. APS March Meeting 2009, Pittsburgh, PA.
- [7] *Dielectric, Piezoelectric and Magnetolectric Properties via First-Principles Calculations at Constant Electric Displacement*. Computational Electronic Structure of Condensed Matter

(CCP9) Conference 2008, Cambridge (UK).

- [6] *First-Principles Modeling of Ferroelectric Capacitors via Calculations at Fixed Electric Displacement Field*. International Symposium on Integrated Ferroelectrics, 2008, Singapore.
- [5] *First-Principles Modeling of Field Effects at Metal-Oxide Heterojunctions*. CECAM Workshop on Maximally Localized Wannier Functions, 2007, Lyon (France).
- [4] *First-principles calculations of nanoscale capacitors at finite bias potential*. APS March Meeting 2007, Denver, CO.
- [3] *First-principles calculations of nanoscale capacitors at finite bias potential*. Workshop on Fundamental Physics of Ferroelectrics 2007, Williamsburg, VA.
- [2] *Origin of the dielectric dead layer in nanoscale capacitors*. Total Energy Conference 2007, Trieste (Italy).
- [1] *Origin of the dielectric dead layer in nanoscale capacitors*. Electronic Structure Conference 2006, Ohio State University, Columbus, OH.

Invited seminars, colloquia and tutorial talks at advanced schools.

- [34] *Natural optical activity from density-functional perturbation theory*. Vanderbilt/Rabe Group Meeting Seminar at Rutgers University. February 27, 2024.
- [33] *First-principles theory and modeling of flexoelectricity in perovskite-based systems*. School on Oxide M/NEMS and Membranes (www.oxinems.eu), online. November 8, 2023.
- [32] *Flexoelectricity and long-range dielectric screening: from 3D to 2D*. News & Views Seminar at ICTP (Trieste). March 7, 2023.
- [31] *First-principles theory of flexoelectricity and related materials properties*. Seminar at ICTP (Trieste). February 6, 2020.
- [30] *New functionalities from gradient couplings: Flexoelectricity and more*. Institute of Physics (IIP), Natal (Brazil). June 2018
- [29] *New functionalities from gradient couplings: Flexoelectricity and more*. TYC Soiree on Multiferroic Materials (London, UK). April 2018.
- [28] *Flexoelectricity from density-functional perturbation theory*. Seminar at Stony Brook University. March 2017.
- [27] *First-principles theory of flexoelectricity*. Seminar at Nanogune (San Sebastián). February 2015.
- [26] *First-principles study of multifunctional perovskite Systems*. RES Engineering Seminar, Barcelona, October 2014.
- [25] *Flexoelectricity via coordinate transformations*. Seminar at the Physics Department, Rutgers University, NJ (USA), March 2014.
- [24] *Flexoelectricity via coordinate transformations*. Seminar at SISSA – Scuola Internazionale Superiore di Studi Avanzati, Trieste (Italy), January 2014.
- [23] *First-principles theory of functional oxide interfaces: From ferroelectric capacitors to confined electron gases*. Seminar at the Max-Planck Institut, Stuttgart (Germany), June 2012.
- [22] *First-principles nanoelectronics: Oxide thin-film devices by design*. Seminar at Technische Universität Darmstadt (Germany), November 2011.
- [21] *Oxides at the nanoscale: Polar interfaces, confined electron gases and more*. Seminar at Materials Theory, ETH Zurich (Switzerland), October 2011.

- [20] *Electrostatics and chemical bonding at metal-ferroelectric interfaces*. Symposium in honour of Alfonso Baldereschi, ITP-EPFL, September 2011.
- [19] *Macroscopic electrostatics at oxide-oxide interfaces: from ferroelectric capacitors to confined electron gases*. Workshop on Advanced Oxide Interfaces, ICTP (Trieste), May 2011.
- [18] *Macroscopic electrostatics at oxide-oxide interfaces: from ferroelectric capacitors to confined electron gases*. Colloquium at the Physics Department, Temple University, PA, April 2011.
- [17] *Macroscopic electrostatics at oxide-oxide interfaces: from ferroelectric capacitors to confined electron gases*. Condensed Matter Physics Seminar (290K), UC Berkeley, March 2011.
- [16] *First-principles modeling of polarity compensation at surfaces and interfaces*. Seminar at CNRS/Thales, Paris, February 2011.
- [15] *First-principles modeling of electrostatically doped perovskite systems*. Colloquium at the ICMAB-CSIC, February 2011.
- [14] *Dielectric, Piezoelectric and Magnetoelectric Properties via First-Principles Calculations at Constant Electric Displacement*. Tutorial talk at AQUIFER School on Multiferroics, L'Aquila, October 2010.
- [13] *First-principles nanoelectronics: Oxide thin-film devices by design*. Seminar at the DPMC, University of Geneva, March 2010.
- [12] *First-principles nanoelectronics: Oxide thin-film devices by design*. Thomas Young Centre Soiree, December 2009.
- [11] *First-principles nanoelectronics: Oxide thin-film devices by design*. Institute of Materials - EPFL, Lausanne, June 2009.
- [10] *First-principles nanoelectronics: Oxide thin-film devices by design*. Argonne CNM Seminar, May 2009.
- [9] *First-principles nanoelectronics: Oxide thin-film devices by design*. Stanford MSE Colloquium, April 2009.
- [8] *Dielectric, Piezoelectric and Magnetoelectric Properties via First-Principles Calculations at Constant Electric Displacement*. Seminar at Universidad de Cantabria, Santander, September 2008.
- [7] *Dielectric, Piezoelectric and Magnetoelectric Properties via First-Principles Calculations at Constant Electric Displacement*. Seminar at ICMAB, Barcelona, September 2008.
- [6] *First-Principles Modeling of Field Effects at Metal-Oxide Heterojunctions*. Argonne MSD Colloquium, Argonne National Lab, IL, September 2007.
- [5] *Origin of the dielectric dead layer in nanoscale capacitors*. Condensed Matter Physics Seminar (290K), UC Berkeley, October 2006.
- [4] *Origin of the dielectric dead layer in nanoscale capacitors*. Materials Colloquium, UCSB, June 2006.
- [3] *Ab-initio theory of nanoscale capacitors at finite bias*. Seminar at the Physics Department, Rutgers University, NJ, May 2006.
- [2] *Accurate polarization with Wannier functions: thin-film capacitors at finite bias*. Seminar at IRRMA, EPFL (Switzerland), October 2005.
- [1] *Ultrathin ionic films on Ag(100): structural and electronic properties*. Electronic Structure Discussion Group, TCM (Cambridge), November 2004.