

Oswaldo Diéguez

Department of Materials Science and Engineering
Faculty of Engineering
Tel Aviv University
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- PERSONAL
- Born in Basel, Switzerland, on 31st March 1972
 - Spanish Citizen
 - Israel Permanent Resident
 - Married to Tal; one daughter (Amalia), one son (Rafael)
- CURRENT EMPLOYMENT
- *Since October 2013*
Senior Lecturer
Tel Aviv University: Department of Materials Science and Engineering
- PAST EMPLOYMENT
- *September 2008 - May 2013*
Scientist (*Ramón y Cajal* Fellow)
Institute of Materials Science of Barcelona (ICMAB-CSIC):
Department of Theory and Computation of Materials
 - *September 2007 – August 2008*
Quantitative analyst
Royal Bank of Scotland, London: Risk Analytics Group
 - *September 2006 – August 2007*
Research associate (supervisor: Prof Nicola Marzari)
MIT: Department of Materials Science and Engineering
 - *April 2003 – August 2006*
Research associate (supervisor: Prof David Vanderbilt)
Rutgers University: Department of Physics and Astronomy
 - *September 2000 – March 2003*
Research associate (supervisor: Prof Mike Payne)
University of Cambridge: Department of Physics, Cavendish Laboratory
- EDUCATION
- *April 2000*
PhD Physics, Universidade de Santiago de Compostela
Dissertation: *Computational Study of Nanoparticles*
Supervisors: Javier Gallego and Carlos Rey
 - *June 1995*
BSc Physics, Universidade de Santiago de Compostela
- HONORS AND AWARDS
- *January 2017*
Outstanding Lecturer in 2015/2016, Faculty of Engineering Dean's List
 - *January 2016*
Outstanding Lecturer in 2014/2015, Faculty of Engineering Dean's List
 - *July 2007*
Awarded a *Ramón y Cajal* Spanish Government excellence contract for 5 years
 - *June 1990*
Honor's Registration to University (university fees waived)

- TEACHING
- Since 2013 (Tel Aviv University)
Physics of Materials (undergraduate)
Introduction to Computational Materials Science (undergraduate)
Atomistic Simulation of Materials (graduate)
 - 2012 (Rutgers University)
General Physics recitations (undergraduate)
 - 2009–2010 (Universitat Autònoma de Barcelona)
Simulation of Materials (graduate)
 - 2007 (MIT)
Atomistic Simulation of Materials computational lab (undergraduate)
 - 2005 (Rutgers University)
General Physics recitations (undergraduate)
 - 2002–2003 (University of Cambridge)
Special Relativity and Electrodynamics supervisions (undergraduate)
Mathematics supervisions (undergraduate)
 - 1998–2000 (Universidade de Santiago de Compostela)
Thermodynamics recitations (undergraduate)
- SUPERVISION
- Eli Zick: PhD Student (10/2018–now); topic: *Calculation of NMR signatures in two-dimensional materials*
 - Avi Auslender: PhD Student (10/2018–now, cosupervised with Prof. Amit Kohn); topic: *Mean inner potential of solids: experiments and calculations*
 - Netanela Cohen: MSc Student (10/2018–now); topic: *Computational discovery of new phases in perovskite oxides*
 - Ronen Kruchinin: MSc Student (06/2018–now); topic: *Density-functional study of catalysis on two-dimensional chalcogenides*
 - Matan Dascalu: PhD Student (10/2014–now, cosupervised with Prof. Ilan Goldfarb); topic: *Experiments and theory of transition metal silicides*
 - Maor Asher: MSc Student (10/2014–01/2018); topic: *Computational studies of electrostrictive materials*
 - Vivek A. Singh: Postdoctoral Fellow (12/2016–09/2018); topic: *Atomistic simulation of ferroelectrics*
 - Akansha Singh: Postdoctoral Fellow (11/2015–09/2018); topic: *Atomistic simulation of multiferroic oxides*
- GRANTS
- *Modeling ferroelectric domain walls from first-principles: interaction with defects and implications for photovoltaics*
Funding Agency: Israel Science Foundation (Individual Research Grant)
Role of Applicant: Principal Investigator (no co-applicants)
Amount Granted: 196,111 NIS/year for 4 years (starting October 2014)
 - *Computational Resources for Computational Materials Modelling*
Funding Agency: Israel Science Foundation (New-Faculty Equipment Grants)
Role of Applicant: Principal Investigator (no co-applicants)
Amount Granted: 213,000 NIS (starting October 2014)
 - *Fundamental studies and computational design of nanostructured functional oxides (MULTIOXIDES)*
Spanish Ministry of Science and Innovation
Amount Granted: €48,000 (2011-2013, shared with Jorge Íñiguez (ICMAB-CSIC) and Massimiliano Stengel (ICMAB-CSIC))

- SERVICE
- Member of the Scientific Committee: *The 17th Israel Materials Engineering Conference*, Bar-Ilan University, 1-2 February 2016
 - Co-organizer: *High-Throughput Materials Discovery: Perspectives and Challenges in Theory and Experiment*, Tel Aviv (Israel), 3-5 February 2016 (international workshop)
 - Co-organizer: *Efficient Density-Functional Calculations with Atomic Orbitals: A Hands-On Tutorial of the Siesta and TranSiesta Codes*, Tel Aviv (Israel), 8-11 September 2014 (international tutorial with around 40 attendees)
 - Seminar Organizer, The Raymond and Beverly Sackler Center for Computational Molecular and Materials Science at Tel Aviv University
 - Representative of the Israel Node at the CECAM Council
 - Committee Member: Physics in the *Materials and Chemistry* undergraduate program
 - Committee Member: Mathematics in the *Materials and Chemistry* undergraduate program
 - Committee Member: Ph.D. Studies Committee, Faculty of Engineering, Tel Aviv University
 - Committee Member: Computers Committee, Faculty of Engineering, Tel Aviv University
 - Grant Proposals Referee: Israel Science Foundation (Israel); Ministry of Science, Technology and Space (Israel); and The PAZY Foundation (Israel).
 - Journal Referee: Physical Review Letters, Physical Review B, Applied Physics Letters, Physica Status Solidi, Phase Transitions, Journal of Applied Crystallography, Applied Physics A

- INVITED TALKS
- *Polymorphism in Bi-based Perovskite Oxides: a First-Principles Study*, Third NU-TAU Workshop: Recent Advances in Materials Science and Engineering, Evanston IL (USA), 16–18 July 2018
 - *Polymorphism in Bi-based Perovskite Oxides: a First-Principles Study*, The Ministry of Science and Technology: Israel-India Workshop, Tel Aviv (Israel), 27 June 2018
 - *Domain Walls in Multiferroic Bismuth Ferrite: An Ab Initio Study*, 14th International Ceramics Congress: CIMTEC 2018, Perugia (Italy), 4–8 June 2018
 - *Polymorphism in Bi-based perovskite oxides: first-principles study*, Fritz Haber Seminar, The Hebrew University of Jerusalem, Jerusalem (Israel), 10 May 2018
 - *Handling Transition Metals in Perovskite Oxides: DFT+U and Hybrid Functionals Results*, Strongly Correlated Materials: Experiments and Computation, Tel Aviv (Israel), 09–12 April 2018
 - *Atomistic simulation of the effect of misfit strain on the properties of epitaxial films: oxides and silicides*, 6th International Workshop: SemiconNano 2017, Como (Italy), 25–28 September 2017
 - *Tailoring the properties of perovskite oxides through epitaxial strain: a first-principles study*, Invited Seminar at the Department of Materials Engineering of Ben Gurion University, Beersheba (Israel), 22 December 2016
 - *Using Strain to Tailor the Properties of Perovskite Oxides: A First-Principles Study*, The Isaiah Shavitt Workshop Series On "Quantum Mechanics in Chemistry: From Structure to Dynamics", Haifa (Israel), 15 December 2016
 - *A SIESTA Tutorial*, Materials Science Codes on Innovative HPC Architectures: Prace-MaX Training, Bologna (Italy), 7 December 2016
 - *The effect of strain in the properties of ferroelectric perovskite oxides: a first-principles study*, Invited THEOS-MARVEL Seminar at the École Polytechnique Fédérale de Lausanne, Lausanne (Switzerland), 24 November 2016

- *Atomistic simulation of ferroelectric and multiferroic perovskite oxides*, "Northwestern University / Tel Aviv University Workshop: Energy, Sustainability, and Biomaterials", Evanston IL (USA), 20 September 2016
- *Inducing ferroic ordering in perovskite oxides through epitaxial strain: first-principles results*, "FUN2025: Functional and Nanomaterials 2025", Irvine CA (USA), 16 September 2016
- *First-Principles Prediction of Supertetragonal Phases in Perovskite Oxide Films: The Case of BiMnO₃*, 27th "Fundamental Physics of Ferroelectrics Workshop", Washington DC (USA), 1 February 2016
- *Ferroelectric films of bismuth ferrite with small band gap: a first-principles study*, XXXIII Israel Vacuum Society Annual Meeting, Rehovot (Israel), 9 September 2015
- *Ferroelectric Domain Walls in Bismuth Ferrite: a First-Principles Study*, The 16th Israel Materials Engineering Conference, Haifa (Israel), 25 February 2014
- *Ferroelectric Domain Walls in Bismuth Ferrite: a First-Principles Study* All Oxide Photovoltaics CECAM Workshop, Jerusalem (Israel), 16 December 2013
- *Domain Walls in a Perovskite Oxide with Two Order Parameters: First-principles Study of BiFeO₃*, XXXI Israel Vacuum Society Annual Meeting, Herzliya (Israel), 30 September 2013
- *Tuning the structure and properties of BiFeO₃ and related materials from first-principles*, JEMS 2012, Parma (Italy), 10-14 September 2012
- *First-principles study of new multiferroic perovskite oxides*, CIMTEC 2012, Montecatini Terme (Italy), 10-14 June 2012
- *Wannier-Based Definition of Layer Polarizations, Maximally Localized Wannier Functions* CECAM Workshop, Lyon (France), 27-29 June 2007
- *First-principles study of epitaxial strain in perovskites*, Novel Materials for Micro- and Nanoelectronics (PASI 2007), Renaca (Chile), 8-18 January 2007
- *Theoretical study of ferroelectric potassium nitrate*, Novel Materials for Micro- and Nanoelectronics (PASI 2007), Renaca (Chile), 8-18 January 2007
- *Mapping of energy versus polarization in ferroelectric materials*, 18th Annual Workshop on Recent Developments in Electronic Structure Methods, Columbus OH (USA), 22-25 June 2006
- *First-principles simulations at constant electric polarization*, 12th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods, Trieste (Italy), 13-15 January 2005
- *Ab initio Study of the Phase Diagram of Epitaxial BaTiO₃*, Laboratory for Surface Modification 18th Annual Symposium, Piscataway NJ (USA), 26 February 2004
- *Ab initio Study of the Phase Diagram of Epitaxial BaTiO₃*, Ferroelectrics 2004, Williamsburg VA (USA), 8-11 February 2004
- *Order-N calculations in metals with the finite temperature method*, Local Orbitals and Linear-scaling Ab Initio Calculations Workshop, Lyon (France), 3-7 September 2001

○ **Citation Metrics:**

Most recent data: <http://www.researcherid.com/rid/C-1386-2009>

— Sum of the Times Cited: 1700+

— h-index: 18

○ **Articles listed in the Web of Knowledge database:**

- [37] M. Asher, and O. Diéguez: *A Computational Study of Gadolinium-Doped Ceria: Relationship between Atomic Arrangement and Electrostriction*; APL Materials 7, 041109 (2019)
- [36] M. Dascalu, F. Cesura, G. Levi, O. Diéguez, A. Kohn, and I. Goldfarb: *Controlling the Supermagnetic Response of Tetragonal α -FeSi₂ Nanoislands*; Applied Surface Science 476, 189 (2019)
- [35] A. Auslender, M. Halabi, G. Levi, O. Diéguez, and A. Kohn: *Measuring the mean inner potential of Al₂O₃ sapphire using off-axis electron holography*; Ultramicroscopy 198, 18 (2019)
- [34] A. Singh, V.N. Singh, E. Canadell, J. Íñiguez, and O. Diéguez: *Polymorphism in Bi-based perovskite oxides: a first-principles study*; Physical Review Materials 2, 104417 (2018)
- [33] L. Zhang, J. Chen, L. Fan, O. Diéguez, J. Cao, Z. Pan, Y. Wang, J. Wang, M. Kim, S. Deng, J. Wang, H. Wang, J. Deng, R. Yu, J.F. Scott, and X. Xing: *Giant Polarization in Super-Tetragonal Thin Films through Interphase Strain*; Science 361, 494 (2018)
- [32] C. Cazorla, O. Diéguez, and J. Íñiguez: *Multiple structural transitions driven by spin-phonon couplings in a perovskite oxide*; Science Advances 3, e1700288 (2017)
- [31] R. Chalasani, A. Pekin, A. Rabkin, R. Abutbul, O. Diéguez, Y. Kauffmann, Y. Golan, and A. Kohn: *Mapping Charge Distribution in Single PbS Core – CdS Arm Nano-Multipod Heterostructures by Off-Axis Electron Holography*; Nano Letters 17, 2778 (2017)
- [30] O. Diéguez and J. Íñiguez: *Multiferroic Bi₂NiMnO₆ thin films: A computational prediction*; Physical Review B 95, 085129 (2017)
- [29] Z. Gareeva, O. Diéguez, J. Íñiguez, and A. Zvezdin, *Interplay between elasticity, ferroelectricity and magnetism at the domain walls of bismuth ferrite*, Phys. Status Solidi RRL 10, 209 (2016)
- [28] O. Diéguez and J. Íñiguez, *Epitaxial phases of BiMnO₃ from first principles*, Phys. Rev. B **91**, 184113 (2015).
- [27] Z. Gareeva, O. Diéguez, J. Íñiguez, and A. Zvezdin, *Complex domain walls in BiFeO₃*, Phys. Rev. B **91**, 060404 (2015).
- [26] W. Ren, Y. Yang, O. Diéguez, J. Íñiguez, N Choudhury, and L. Bellaiche, *Ferroelectric domains in multiferroic BiFeO₃ films under epitaxial strain*, Phys. Rev. Lett. **110**, 187601 (2013).
- [25] O. Diéguez, P. Aguado-Puente, J. Junquera, and J. Íñiguez, *Domain walls in a perovskite oxide with two primary structural order parameters: First-principles study of BiFeO₃*, Phys. Rev. B **87**, 024102 (2013)
- [24] C. Escorihuela-Sayalero, O. Diéguez, and J. Íñiguez, *Strain engineering magnetic frustration in perovskite oxide thin films*, Phys. Rev. Lett. **109**, 247202 (2012)
- [23] O.E. González-Vázquez, J. Wojdeł, O. Diéguez, and J. Íñiguez, *First-principles investigation of the structural phases and enhanced response properties of the BiFeO₃-LaFeO₃ multiferroic solid solution*, Phys. Rev. B **85**, 064119 (2012)
- [22] I.C. Infante, J. Juraszek, S. Fusil, B. Dupè, P. Gemeiner, O. Diéguez, et al., *Multiferroic phase transition near room temperature in BiFeO₃ thin films*, Phys. Rev. Lett. **107**, 237601 (2011)

- [21] O. Diéguez and J. Íñiguez, *First-principles investigation of morphotropic transitions and phase-change functional responses in BiFeO₃-BiCoO₃ multiferroic solid solutions*, Phys. Rev. Lett. **107**, 057601 (2011)
- [20] O. Diéguez, O.E. González-Vázquez, J. Wojdeł, and J. Íñiguez, *First-principles predictions of low-energy phases of multiferroic BiFeO₃*, Phys. Rev. B **83**, 094105 (2011)
- [19] O. Diéguez and N. Marzari *First-principles characterization of the structure and electronic structure of alpha-S and Rh-S chalcogenides*, Phys. Rev. B **80**, 214115 (2009)
- [18] O. Diéguez and D. Vanderbilt, *First-principles modeling of strain in perovskite ferroelectric thin films*, Phase Transit. **81**, 607 (2008)
- [17] E. Artacho, E. Anglada, O. Diéguez, J. D. Gale, A. García, *et al.*, *The SIESTA method; developments and applicability*, J. Phys. Condens. Mat. **20**, 064208 (2008)
- [16] O. Diéguez and D. Vanderbilt, *Theoretical study of ferroelectric potassium nitrate*, Phys. Rev. B **76**, 134101 (2007)
- [15] R. C. Longo, E. Martínez, O. Diéguez, A Vega, and L. J. Gallego, *Morphology and magnetism of Fe monolayers and small Fe_n clusters (n = 2-19) supported on the Ni(111) surface*, Nanotechnology **18**, 055701 (2007)
- [14] X. Wu, O. Diéguez, K. M. Rabe, and D. Vanderbilt, *Wannier-based definition of layer polarizations in perovskite superlattices*, Phys. Rev. Lett. **97**, 107602 (2006)
- [13] O. Diéguez and D. Vanderbilt, *First-principles simulations at constant electric polarization*, Phys. Rev. Lett. **96**, 056401 (2006)
- [12] O. Diéguez, R. C. Longo, A. Vega, and L. J. Gallego, *Structure of a Fe monolayer supported on the Ni (111) surface. A density-functional theory study using the generalized gradient approximation*, Solid State Comm. **137**, 129 (2006)
- [11] O. Diéguez, K. M. Rabe, and D. Vanderbilt, *First-principles study of epitaxial perovskites*, Phys. Rev. B **72**, 144101 (2005)
- [10] O. Diéguez, S. Tinte, A. Antons, C. Bungaro, J. B. Neaton, *et al.*, *Ab initio Study of the Phase Diagram of Epitaxial BaTiO₃*, Phys. Rev. B **69**, 212101 (2004)
- [9] C. K. Skylaris, O. Diéguez, P. D. Haynes, and M. C. Payne, *Comparison of variational real-space representations of the kinetic energy operator*, Phys. Rev. B **66**, 073103 (2002)
- [8] C. K. Skylaris, A. A. Mostofi, P. D. Haynes, O. Diéguez, and M. C. Payne, *The Non-orthogonal Generalised Wannier Function pseudopotential plane-wave method*, Phys. Rev. B **66**, 035119 (2002)
- [7] O. Diéguez, M. M. G. Alemany, C. Rey, P. Ordejón, and L. J. Gallego, *Ab initio density-functional calculations of the structures, binding energies and magnetic moments of Fe clusters with 2 to 17 atoms*, Phys. Rev. B **63**, 205407 (2001)
- [6] M. M. G. Alemany, O. Diéguez, C. Rey, and L. J. Gallego, *A density-functional study of the structures and electronic properties of C₅₉Ni and C₆₀Ni clusters*, J. Chem. Phys. **114**, 9371 (2001)
- [5] C. Rey, M. M. G. Alemany, O. Diéguez and L. J. Gallego, *Ab initio density-functional calculations of the geometries, electronic structures and magnetic moments of Ni-C clusters*, Phys. Rev. B **62**, 12 640 (2000)
- [4] M. M. G. Alemany, C. Rey, O. Diéguez and L. J. Gallego, *A computer simulation study of the static structure and dynamic properties of liquid C₆₀ using Girifalco's potential*, J. Chem. Phys. **112**, 10711 (2000)
- [3] R. C. Longo, O. Diéguez, C. Rey and L. J. Gallego, *Embedded atom model calculations of the structures of small Ni clusters and of a full Ni monolayer on the (001) surface of Al*, Eur. Phys. J. D **9**, 543 (1999)

- [2] O. Diéguez, R. C. Longo, C. Rey and L. J. Gallego, *A computer simulation study of the ground-state configurations of Fe and Fe-Al clusters*, Eur. Phys. J. D **7**, 573 (1999)
- [1] M. M. G. Alemany, O. Diéguez, C. Rey and L. J. Gallego, *Molecular-dynamics study of the dynamic properties of fcc transition and simple metals in the liquid phase using the second-moment approximation to the tight-binding method*, Phys. Rev. B **60**, 9208 (1999)
- **Articles published as book chapters:**
- [1] C. Rey, J. García-Rodeja, O. Diéguez, and L. J. Gallego, *A tight binding molecular dynamics study of the structures and melting of hcp transition metals*, in *Non-crystalline and Nanoscale Materials*, edited by J. Rivas and M. A. López-Quintela (World Scientific, Singapore, 1998)