Oswaldo Diéguez

Department of Materials Science and Engineering
Faculty of Engineering
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PERSONAL

- Born in Basel, Switzerland, on 31st March 1972
- Spanish citizen
- Israel Work Permit: A5 (temporary residence visa)
- 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 Governmnet 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

- Vivek A. Singh: Postdoctoral Fellow, starting December 2016; topic: *atomistic simulation of ferroelectrics*
- Akansha Singh: Postdoctoral Fellow, starting November 2015; topic: *atomistic simulation of multiferroic oxides*
- Matan Dascalu: PhD Student, starting October 2014 (in collaboration with Prof. Ilan Goldfarb); topic: *experiments and theory of transition metal silicides*
- Maor Asher: MSc Student, starting October 2014; topic: *computational studies of electrostrictive materials*
- Carlos Escorihuela-Sayalero (2012): Cosupervised final-year undergraduate project, *strain engineering magnetic frustration in perovskite oxide thin films*
- Carlos Escorihuela-Sayalero (2011): Supervised summer undergraduate internship, *A tight-binding method for carbon*

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))
- *First-principles study of ferroelectrics and multiferroics*
  Spanish Supercomputing Network
  Amount Granted: 1,350,000 hours of supercomputing time (2009-2013)
- *First-principles study of advanced materials*
  Ramón y Cajal start-up funding, Spanish Ministry of Science and Innovation
  Amount Granted: €15,000 (2008-2010)

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

- *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 $BiMnO_3$*, 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 $BiFeO_3$*, XXXI Israel Vacuum Society Annual Meeting, Herzliya (Israel), 30 September 2013
- *Tuning the structure and properties of $BiFeO_3$ 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 $BaTiO_3$*, Laboratory for Surface Modification 18th Annual Symposium, Piscataway NJ (USA), 26 February 2004
- Ab initio *Study of the Phase Diagram of Epitaxial $BaTiO_3$*, 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

PUBLICATIONS

- **Citation Metrics:**

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

  — Sum of the Times Cited: 1300+

  — h-index: 17

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

[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 $BiMnO_3$ from first principles*, Phys. Rev. B **91**, 184113 (2015).

[27] Z. Gareeva, O. Diéguez, J. Íñiguez, and A. Zvezdin, *Complex domain walls in $BiFeO_3$*, Phys. Rev. B **91**, 060404 (2015).

[26] W. Ren, Y. Yang, O. Diéguez, J. Íñiguez, N Choudhury, and L. Bellaiche, *Ferroelectric domains in multiferroic $BiFeO_3$ 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 $BiFeO_3$*, 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 $BiFeO_3$-$LaFeO_3$ 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 $BiFeO_3$ 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 $BiFeO_3$-$BiCoO_3$ 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 $BiFeO_3$*, 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 $BaTiO_3$*, 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 $C_{59}Ni$ and $C_{60}Ni$ 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 C_{60} 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)