

## Curriculum Vitae – Jorge Íñiguez

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*Mar. 2003-:* Postdoctoral fellow at the University of Maryland & NIST (USA)  
working with Dr. Taner Yildirim (NIST).  
*2001-2003:* Postdoctoral fellow at Rutgers University (USA)  
working in Prof. David Vanderbilt's group.  
*Feb. 2001:* PhD. in Physics at the Universidad del País Vasco (Spain).  
Thesis title: *ab-initio calculations and effective Hamiltonians  
for the study of ferroelectric materials*  
Supervisors: Prof. Alberto García and Prof. J.M. Pérez-Mato  
*Fall 2000:* Visiting scientist at the University of Arkansas (USA)  
working in Prof. Laurent Bellaïche's group  
*1997-2001:* PhD. Student in Materials Science  
at the Universidad del País Vasco (Spain)  
*1996-1997:* Predoctoral research at the Universidad del País Vasco (Spain)  
Supervisor: Prof. Ana Achúcarro

*Education at the Universidad del País Vasco (Spain)*

*1997-1998:* Post-graduate courses in Materials Science.

*1992-1997:* Master degree in Physics,  
awarded First Prize for graduating Physics majors.

## OVERVIEW OF RESEARCH ACTIVITIES

1. *First-principles studies of ferroelectric materials.*  
My work has ranged from essentially methodological issues [23,13,8] to the solution of long-standing problems such as the temperature-pressure phase diagram of BaTiO<sub>3</sub> [11].
2. *First-principles study and design of piezoelectric alloys*  
My work has ranged from the study of technologically important, poorly understood piezoelectric alloys [7,6] to the computer design of piezoelectric perovskite solid solutions with optimum (predetermined) properties [17,16].
3. *Structural phase transitions.*  
Three examples are: the development of an efficient method to calculate free-energy Landau potentials out of statistical simulations [18], the prediction of pressure-induced sequences of quantum phase transitions [11] and the prediction of short-range order induced phase transitions in piezoelectric alloys [6].
4. *Development of new Density Functional Theory (DFT) methods.*  
Ivo Souza, David Vanderbilt and I have recently proposed an efficient way to perform first-principles calculations of insulators in finite, homogeneous, static or time-dependent electric fields [10,5].
5. *Computational crystallography* [22,19,20].
6. *Modelization of amorphization induced by pressure* [14,12].
7. **Current work includes:** lattice dynamics of various systems (studies combining first-principles and neutron scattering [3]), strongly-correlated systems [1], non-collinear magnetism, protonic conductors, quantum paraelectrics and relaxors [4], etc.

## LIST OF SCIENTIFIC PUBLICATIONS

(in reverse chronological order)

1. *Unusual structural tuning of magnetism in cuprate perovskites*, Jorge Íñiguez and Taner Yildirim (submitted).
2. *Orbital and spin chains in  $ZnV_2O_4$* , S.-H. Lee, D. Louca, H. Ueda, S. Park, T.J. Sato, M. Isobe, Y. Ueda, S. Rosenkranz, P. Zschack, Jorge Íñiguez, Y. Qiu and R. Osborn (submitted).
3. *Structure and hydrogen dynamics of pure and Ti-doped sodium alanate*, Jorge Íñiguez, Taner Yildirim, T.J. Udovic, M. Sulic and C.M. Jensen, Physical Review B (RC) 70, 060101 (2004).
4. *Atomistic simulations of the incipient ferroelectric  $KTaO_3$* , A.R. Akbarzadeh, L. Bellaiche, Kevin Leung, Jorge Íñiguez and David Vanderbilt (Physical Review B, in press).
5. *Dynamics of Berry-phase polarization in time-dependent electric fields*, Ivo Souza, Jorge Íñiguez, and David Vanderbilt, Physical Review B 69, 085106 (2004).
6. *Effects of atomic short-range order on the properties of perovskite alloys in the morphotropic phase boundary*, A. M. George, Jorge Íñiguez, and L. Bellaiche, Physical Review Letters 91, 045504 (2003).
7. *First-principles study of  $(BiScO_3)_{1-x} - (PbTiO_3)_x$  piezoelectric alloys*, Jorge Íñiguez, D. Vanderbilt, and L. Bellaiche, Physical Review B 67, 224107 (2003).
8. *Quantitative analysis of the first-principles effective Hamiltonian approach to ferroelectric perovskites*, Silvia Tinte, Jorge Íñiguez, Karin M. Rabe, and D. Vanderbilt, Physical Review B 67, 064106 (2003).
9. *Thermally diluted Ising systems*, Manuel I. Marqués, Julio A. Gonzalo, and Jorge Íñiguez, Fractals 11 Suppl., 53 (2003).
10. *A first-principles approach to insulators in finite electric fields*, Ivo Souza, Jorge Íñiguez, and D. Vanderbilt, Physical Review Letters 89, 117602 (2002).

11. *First-principles study of the temperature-pressure phase diagram of BaTiO<sub>3</sub>*, Jorge Íñiguez and D. Vanderbilt, Physical Review Letters 89, 115503 (2002).
12. *Pressure amorphization through displacive disorder*, Morrel H. Cohen, Jorge Íñiguez, and J.B. Neaton, The European Physical Journal E 9, 239-243 (2002).
13. *Effective-Hamiltonian modeling of external pressures in ferroelectric perovskites*, Jorge Íñiguez, J.B. Neaton, and D. Vanderbilt, *Fundamental Physics of Ferroelectrics, 2002*, R. E. Cohen, ed. (AIP, Melville, New York, 2002), p. 56.
14. *Flat branches and pressure amorphization*, M.H. Cohen, Jorge Íñiguez, and J.B. Neaton, Journal of Non-Crystalline Solids vol. 307-310, 602 (2002).
15. *Optical phonons associated with the low-temperature ferroelectric properties of perovskite solid solutions*, A.M. George, Jorge Íñiguez, and L. Bellaiche, Physical Review B (RC) 65, 180301 (2002).
16. *Atomic-ordering induced anomalous properties in ferroelectrics*, A.M. George, Jorge Íñiguez, and L. Bellaiche, Nature 413, 54 (2001).
17. *Ab-initio design of perovskite alloys with predetermined properties: The case of Pb(Sc<sub>0.5</sub>Nb<sub>0.5</sub>)O<sub>3</sub>*, Jorge Íñiguez and L. Bellaiche, Physical Review Letters 87, 095503 (2001).
18. *Ab initio Devonshire-Landau free energy of BaTiO<sub>3</sub>*, Jorge Íñiguez, S. Ivantchev, J. M. Pérez-Mato, and Alberto García, Physical Review B 63, 144103 (2001).
19. *Local mode transferability from cubic perovskite to hexagonal barium titanate*, Jorge Íñiguez, Alberto Garcia, and J.M. Perez-Mato, *Fundamental Physics of Ferroelectrics, 2000*, R. E. Cohen, ed. (AIP, Melville, New York, 2000), p. 88.
20. *Analysis of soft optical modes in hexagonal BaTiO<sub>3</sub>: transference of perovskite local distortions*, Jorge Íñiguez, Alberto Garcia, and J.M. Perez-Mato, Journal of Physics: Condensed Matter 12, L387 (2000).

21. *Universality class of thermally diluted Ising systems at criticality*, Manuel I. Marqués, Julio A. Gonzalo, and Jorge Íñiguez, Physical Review E 62, 191 (2000).
22. *First-principles study of the structural instabilities of hexagonal barium titanate: coupling between the soft optical and the acoustic modes*, Jorge Íñiguez, Alberto Garcia, and J.M. Perez-Mato, Ferroelectrics 237 (1-4), 329-336 (2000).
23. *Optimized local modes for lattice-dynamical applications*, Jorge Íñiguez, Alberto Garcia, and J.M. Perez-Mato, Physical Review B (BR) 61, 3127 (2000).

## SCIENTIFIC MEETINGS ATTENDED

(in reverse chronological order)

1. 2nd American Conference on Neutron Scattering, in College Park (USA), June 2004.
2. 16th Annual Workshop on Recent Developments in Electronic Structure Methods, in New Brunswick (USA), May 2004.
3. 2004 March Meeting of the American Physical Society, in Montreal (Canada), March 2004.
4. “Theory, Modeling, and Neutron Scattering for Study of Advanced Materials” workshop, in Gaithersburg (USA), August 2003.
5. XI International workshop on computational physics and materials science: Total energy and force methods, in Trieste (Italy), January 2003.
6. 2002 March Meeting of the American Physical Society, in Indianapolis (USA), March 2002.
7. “Fundamental Physics of Ferroelectrics 2002” workshop, in Washington D.C. (USA), February 2002.
8. “Thermodynamic and Structural Properties of Materials” workshop, in Avignon (France), September 2001.
9. 10th International Meeting on Ferroelectricity, in Madrid (Spain), September 2001.
10. ES2001 – Thirteenth Annual Workshop on Recent Developments in Electronic Structure Algorithms, in Princeton (USA), June 2001.
11. 2001 March Meeting of the American Physical Society, in Seattle (USA), March 2001.
12. 2000 “Electronic structure approaches to the physics of materials” Spring college, in ICTP, Trieste (Italy), May-June 2000.
13. “Fundamental Physics of Ferroelectrics 2000” workshop, in Aspen (USA), February 2000.

14. SPAIN-2000 MINI-WORKSHOP on Advances in first-principles computational condensed matter physics, in Madrid (Spain), January 2000.
15. 9th European Meeting on Ferroelectricity, in Prague (Czech Republic), July 1999.
16. “Condensed matter physics: applications of the density functional theory and methods of quantum chemistry” workshop, in Laredo (Spain), July 1999.

## SELECTED PRESENTATIONS IN SCIENTIFIC MEETINGS

(in reverse chronological order)

1. Invited talk at the 2nd American Conference on Neutron Scattering, in College Park (USA), 2004; *Multiphonon scattering and hydrogen dynamics in pure and Ti-doped sodium alanate*.
2. Poster at the 16th Annual Workshop on Recent Developments in Electronic Structure Methods, in New Brunswick (USA), 2004; Jorge Íñiguez and Taner Yildirim; *Interplay between structure and magnetism in  $\text{Se}_{1-x}\text{Te}_x\text{CuO}_3$  alloys*.
3. Contributed talk at the 2004 March Meeting of the American Physical Society, in Montreal (Canada), 2004; Jorge Íñiguez and Taner Yildirim; *“Towards the first-principles design of materials with tailored magnetic properties”*.
4. Contributed talk at the 2004 March Meeting of the American Physical Society, in Montreal (Canada), 2004; Taner Yildirim and Jorge Íñiguez; *“Combined first-principles modeling and neutron scattering characterization of hydrogen storage materials”*.
5. Contributed talk at the 2003 March Meeting of the American Physical Society, in Austin (USA), 2003; Jorge Íñiguez, David Vanderbilt, and L. Bellaiche; *“First principles study of  $(\text{BiScO}_3)_x - (\text{PbTiO}_3)_{1-x}$  piezoelectric alloys”*.
6. Contributed talk at “Fundamental Physics of Ferroelectrics, 2003”, in Williamsburg (USA), 2003; Jorge Íñiguez, David Vanderbilt, and L. Bellaiche; *“First principles study of  $(\text{BiScO}_3)_x - (\text{PbTiO}_3)_{1-x}$  piezoelectric alloys”*.
7. Invited talk at the XI International workshop on computational physics and materials science: Total energy and force methods, in Trieste (Italy), 2003; *“First-principles approach to insulators in finite electric fields”*.
8. Contributed talk at the 2002 March Meeting of the American Physical Society, in Indianapolis (USA), 2002; Jorge Íñiguez and D. Vanderbilt; *“First-principles study of the temperature-pressure phase diagram of  $\text{BaTiO}_3$ ”*.

9. Contributed talk at “Fundamental Physics of Ferroelectrics, 2002”, in Washington D.C. (USA), 2002; Jorge Íñiguez and D. Vanderbilt; “*First-principles study of the temperature-pressure phase diagram of BaTiO<sub>3</sub>*”.
10. Invited talk at “Thermodynamic and Structural Properties of Materials”, in Avignon (France), 2001; “*Developments on the effective-Hamiltonian simulation of phase transitions*”.
11. Invited talk at the 10th International Meeting on Ferroelectricity, in Madrid (Spain), 2001; Jorge Íñiguez, L. Bellaiche, David Vanderbilt, A. García, S. Ivantchev and J. M. Pérez-Mato, “*Recent developments in ab-initio calculations in ferroelectrics with effective Hamiltonians*”.
12. Poster at the ES2001 - Thirteenth Annual Workshop on Recent Developments in Electronic Structure Algorithms, in Princeton (USA), 2001; Ivo Souza, Jorge Íñiguez, and David Vanderbilt, “*k-space treatment of insulators in finite electric fields*”.
13. Contributed talk at the 2001 March Meeting of the American Physical Society, in Seattle (USA), 2001; Jorge Íñiguez, S. Ivantchev, J.M. Pérez-Mato, and Alberto García, “*Ab initio Devonshire-Landau free energy of BaTiO<sub>3</sub>*”.
14. Talk at the 2000 Spring College on Electronic Structure Approaches to the Physics of Materials, ICTP, Trieste (Italy), 2000; “*Analysis of soft optical modes in hexagonal BaTiO<sub>3</sub>: transference of perovskite local distortions*”.
15. Poster at the 2000 Workshop on Fundamental Physics of Ferroelectrics, in Aspen (USA), 2000; Jorge Íñiguez, Alberto García, and J. M. Pérez-Mato, “*Local mode transferability from cubic perovskite to hexagonal barium titanate*”.
16. Poster at the 9th European Meeting on Ferroelectricity, in Prague (Czech Republic), 1999; Jorge Íñiguez, A. García, and J. M. Pérez-Mato, “*First-Principles Study Of The Structural Instabilities Of Hexagonal Barium Titanate: Coupling Between The Soft Optical And The Acoustic Modes*”.

## REFERENCES

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