Curriculum Vitae

Tomás Alberto Arias, Ph.D.
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BIRTH

July 19, 1964, Philadelphia, Pennsylvania. Citizen of United States of America.

EDUCATION

- **Doctor of Philosophy in Physics**, MIT, *1992*
  Thesis: *New Analytic and computational techniques for finite temperature condensed matter systems.*
- **Bachelor of Science in Physics**, MIT, *1986*
  Thesis: *Modulated Spectral Activity in Jovian radio emissions.*
- **High School Diploma**, Abington Senior High School, Pennsylvania, *1982*

ACADEMIC APPOINTMENTS

- **Full Professor**, Department of Physics, Cornell University, *July 2005 – present*
- **Associate Professor**, Department of Physics, Cornell University, *July 1999 – June 2005*
- **Research Affiliate**, Research Laboratory of Electronics, MIT, *July 1999 – July 2001*
- **Associate Professor**, Department of Physics, MIT, *July 1999*
- **Assistant Professor**, Department of Physics, MIT, *1993–1999*
- **Post Doctoral Associate**, Department of Physics, MIT, *1992–1993*
- **Graduate Research Assistant**, Department of Physics, MIT, *1988–1992*
- **Research Associate**, Bell Laboratories, Murray Hill, NJ, *Summer 1987*
- **Graduate Student Instructor**, MIT Experimental Studies Group, *1986–1987*
- **Research Associate**, Bell Laboratories, Murray Hill, NJ, *Summer 1986*
- **Undergraduate Research Assistant**, MIT, *1984–1986*

- **Undergraduate Student Instructor**, MIT Experimental Studies Group, *1983–1984*

AWARDS AND HONORS

- Faculty Fellow, Cornell Center for a Sustainable Future (www.ccsf.cornell.edu) (2009).
- Society for Industrial and Applied Mathematics (SIAM) Outstanding Paper Prize (2001).
- Selected for APS Public Face for Physics (PFP) program (1998).
- MIT School of Science Undergraduate Teaching Prize (1997).
- Department of Energy Defense Programs Young Scientist (1996).
- Alfred P. Sloan Foundation Research Fellow (1995).
- Eugene Sullivan Award for work in theoretical physics (Corning Glass Works,1993).
- MIT Andrew Moore Lockett III Award for excellence in theoretical physics (1990).
- Elected to Sigma Xi (1986).
- AT&T Cooperative Research Fellow (1986).
- Attained highest possible undergraduate GPA at MIT (1986).
- Elected to Phi Beta Kappa; Sigma Pi Sigma (1986).
- Offered MIT Applied Mathematics Fellowship (1986).
- High school: Graduated in top 4% of class; Rensselaer Medal for Science; Philadelphia Science Council Award (Third Place); Best Physics Student of the Year; Elected to National High School Honor Society; John Walton Memorial Award for excellence in music (Junior High).

BIOSKETCH

I am named after my great-grandfather, one of the seven founding fathers of the Republic of Panama and a signer of the Panamanian declaration of independence. I was born in Philadelphia in 1964, and I grew up just north of the city in Abington Township. After receiving my high school diploma from Abington Senior High in 1982, I studied physics at MIT and received my undergraduate degree in 1986. I then continued on at MIT to complete my PhD in 1992 and a short post-doctoral position before joining the faculty there in 1993. In the summer of 1999, I accepted an appointment in the Department of Physics at Cornell University. Settling in New York State, I met my wife, and together we have two daughters. Apart from computers, mathematics and physics, I enjoy photography, exploring the rain forests of Panama, popular cinema, rollerblading, and especially spending time with my wife and daughters.

RESEARCH EXPERIENCE

Professor of Physics, Cornell University, *July 2005 — present*

- Further developments in joint density-functional theory (JDFT); greatly improved functionals for dipolar fluids based on exact analytic treatment of the non-interacting molecular system.
- Application of JDFT to electrochemistry
- *Ab initio*, continuum many-body exploration of losses in carbon nanotube systems
- Excited state studies in molecular organic materials
- Experimentally confirmed predictions of properties of point and planar defects in perovskite materials

Associated Professor of Physics, Cornell University, *July 1999 — July 2005*

- Development of wavelet methods from a promising approach demonstrated only for atoms and diatomic molecules (while at MIT) to an efficient method for high-precision all-electron calculations in solids with unprecedented systematic control over numerical errors.
- *Ab initio* study of materials at high pressures, a new regime of condensed matter physics opened by the advent of the diamond anvil cell.
- Development of a new form of density-functional theory, joint density-functional theory (JDFT), which treats quantum systems in solution rigorously in terms of a "classical" molecular density-functional for the solvent, a Kohn-Sham electron density-functional for the solute, and a universal functional capturing the relevant interactions.
- Application of joint density-functional theory (JDFT) to corrosion of stainless steel alloys.
- Development of rigorous treatments of elasticity on the nanoscale and application of such to tunable carbon nanotube electromechanical oscillators with first identification of all relevant physical regimes (bending dominated, hanging chain, extension dominated).
- First *ab initio* calculation of anelasticity (internal friction) in a material.
- Study of mechanical energy-loss mechanisms in nanoscale oscillators, including atmospheric drag, phonon-phonon and electron-phonon losses in carbon nanotube oscillators.
- *Ab initio* molecular dynamics study of energetic, non-equilibrium crystal growth with first discovery of the importance of internal cluster temperature during pulsed laser deposition.
- First accurate *ab initio* prediction of hyperfine ESR splittings in $C_{59}N$, underscoring uncontrolled errors inherent in non-systematic bases such as Gaussians and need for a truly systematic approach such as wavelets.
- Development of first density-matrix functional to compete with best available gradient-corrected density functionals for electronic structure calculation.
- *Ab initio* prediction of dislocation yield stresses in bcc metals and development of first approach to calculating such from within periodic boundary conditions.
- Discovery of pressure-driven phase transition in grain boundary interactions with vacancies in bcc metals.

Assistant Professor of Physics, MIT, *September 1993 — July 1999.*
<u>FULL–TIME FACULTY WORK AT MIT. JULY 1994 — PRESENT</u>:

- Development of "DFT++," an approach to electronic structure calculations based on a novel basis-set independent formulation of density functional theory.
- Study and development of new energy functionals for density functional theory based upon the quantum mechanical density-matrix.
- *Ab initio* study of the corrosion process of industrial alloys.
- Application of *ab initio* methods to study molecular reactions in solution.
- Local spin-density extension of the Stoner theory of ferromagnetism to explore the microscopic connection between the exchange interaction and inter-granular cohesion in iron.
- Study of grain boundaries and dislocations in molybdenum (an intrinsically brittle bcc metal) and tantalum (a ductile bcc metal).
- Development of multiscale techniques for accelerating *ab initio* thermodynamic calculations through the use of information from atomistic models.
- Identification of the ESR R-center of plastically deformed silicon as the solitons of the 30 degree partial dislocation core.
- Development of fast algorithms for physical operators in wavelet bases for use with electronic structure calculations.
- Investigated specialized, "geometrically correct," minimization techniques on manifolds for application to electronic structure calculations.
- Application of quantum calculations to mechanical properties of nanoscale structures in silicon.

<u>RESEARCH LEAVE — LASSP, CORNELL UNIVERSITY. 1993–1994 ACADEMIC YEAR</u>:

- Application of parallel computation to calculate, at the quantum level, the core energy of and near field interactions among $\langle 110 \rangle$ screw dislocations in silicon.
- Development of formalism and functional code for full–blown, *wavelet*–based first principles' quantum calculations on atoms and diatomic molecules.
- Tailoring special minimization techniques to the Stiefel manifold of orthogonal wave functions in density functional calculations.

Post Doctoral Associate, MIT. *June 1992 — September 1993.*
<u>WORK SUPPORTED BY PROFESSOR JOHN D. JOANNOPOULOS</u>:

- Intensive experience developing massively parallel computation for performing *ab initio* studies of atomic systems large enough to be of fundamental materials interest.

- Exploratory study of the applicability of dynamically adaptive meshes in electronic structure calculations.

- Application of *ab initio* computational techniques to the rigorous theoretical interpretation of experimental Scanning Tunneling Microscopic images of the (110) surface of GaAs.

- *Ab initio* study of the kinetic effects of annealing on the non-equilibrium distribution of point defects on the Si (100) surface.

- Initial, exploratory study of the applicability of wavelet bases for electronic structure calculations.

Research Assistant, MIT. *January 1988 — June 1992.*
<u>Graduate work with Professor John D. Joannopoulos</u>:

- Study of grain boundaries and new dopant segregation mechanisms in elemental semiconductors; establishment of link between carrier trapping and dopant segregation.

- Investigation of the superconducting transition in the Bose gas.

- Development of technique for constrained minimization particularly suited for electronic structure calculations on systems with length–scales beyond 50Å (long enough to begin to be of realistic materials interest).

- Development of *ab initio* quantum molecular dynamics technique that permits, for the first time, finite temperature simulations of long length–scale (∼50Å) systems.

- Development of visualization techniques for the results of *ab initio* material science calculations, in collaboration with the Veridical Users Group at IBM T.J. Watson Research Center.

Research Associate, Bell Laboratories, Murray Hill, NJ. *June 1987 — September 1987.*
<u>Summer position with Dr. Andrew Bobek</u>:

- Development of theory for the effects of materials fluctuations on semiconductor laser performance.

Research Associate, Bell Laboratories, Murray Hill, NJ. *June 1986 — September 1986.*
<u>Summer position with Dr. Ronald J. Schutz</u>:

- Development of computer model of plasma etch processing of electronic devices.

Undergraduate Research Assistant, MIT. *June 1984 — June 1986.*
<u>Undergraduate research with Professor David Staelin</u>:

- Discovery of new form of radio emission from Jupiter using data from the Voyager spacecraft.

RESEARCH INTEREST

My research interest is in developing the science of linking the *ab initio* quantum mechanical description of materials to the behavior of real materials, with emphasis on uncovering fundamental physical issues in systems of potential technological interest. This involves (1) the identification of problems where the quantum perspective can make a significant impact, (2) the exploitation of theoretical techniques and supercomputer architectures to carry out large scale quantum calculations, and (3) the development of new theoretical techniques to link *ab initio* calculations with phenomena on larger scales.

TEACHING EXPERIENCE

- Physics 1101/1102 (Cornell) – Autotutorial Introductory Physics.
  Co-Lecturer: Fall 2007, Spring 2008, Main Lecturer: Fall 2008 – Spring 2010
- Physics 480/680 (Cornell) – Computational Physics.
  Main Lectures: Spring 2001, 2002, 2004, 2005, 2006.
- Physics 214 (Cornell) – Physics III: Optics, Waves, and Particles.
  Recitations: Fall 1999; Main Lectures: Fall 2000, 2001, 2003, 2004, 2005.
- 8.022 (MIT) – Electricity and Magnetism I for advanced students.
  Recitations: Spring 1999.
- 8.012 (MIT) – Mechanics I for advanced students (MIT).
  Recitations: Fall 1998.
- 8.04 (MIT) – Quantum Physics I.
  Recitations: Fall 1994; Main Lectures: Spring 1995, 1996, 1997.
- 8.02 (MIT) – Electricity and Magnetism I.
  Recitations: Spring 1998.
- 8.01 (MIT) – Mechanics I.
  Class Lectures: Fall 1995, 1996.

I developed an award-winning, web-based undergraduate course in quantum mechanics (MIT 8.04) which includes (a) the introduction of Feynman diagrams and renormalization at the undergraduate level, (b) class notes detailing connections between the classic experiments and the theory of wave function representations and operators from a synthetic perspective, and (c) problem sets based on interactive software. See http://www.ccmr.cornell.edu/~muchomas/8.04 .

I have also developed a novel computational physics class (Cornell Phys 480/680) in which senior undergraduate and graduate students construct from scratch their own, fully functional density-functional software for atoms, molecules and solids while learning most of the basic numerical methods as well as high-performance code-optimization techniques.

COMMITTEES

- Member, *Ad hoc* Committee on Introductory Physics Curriculum, *Fall 2009–Spring 2010*.
- Faculty advisor for Cornell Department of Physics Educational Computing *2001—present*.
- Chair, Cornell Physics Graduate Admissions Committee *2004—2008*.
- Co-organizer and host for 17^{th} Annual Workshop on Recent Developments in Electronic Structure Methods, Cornell, *2005*.
- Chair, Review team for DOE advanced scientific computing initiative (ASCI) center at University of Utah, *2004*.
- Member, Cornell Physics Graduate Admissions Committee *2003-2004*.
- Chair, review team for DOE advanced scientific computing initiative (ASCI) center at University of Utah, *2001*.
- Member, review team for DOE advanced scientific computing initiative (ASCI) center at University of Utah, *2000*.
- Faculty Advisor for the Cornell CCMR Research Computing Facility, *2000—present*.
- Chair, Cornell LASSP Theory Seminar Series *1999-2000*.
- Member, review teams for DOE advanced scientific computing initiative (ASCI) center at University of Utah and Caltech, *1999*.
- Symposium Organizer for Fall Meeting: Materials Research Society, *1998-1999*.
- Committee on Education: MIT Department of Physics, *1997*.
- Doctoral General Exam Committee: MIT Department of Physics, *1996-1998*.
- Graduate Admissions Committee: MIT Department of Physics, *1996-1997*.
- Institute Committee on Student Affairs: MIT, *1994-1995*.

Physics Educational Computing Cluster — While serving as the faculty advisor for physics educational computing at Cornell, I initiated a new model for the department's undergraduate and graduate educational computing resources based upon open software and cluster computing, oversaw a complete overhaul of the computing facility, and hold introductory seminars for incoming students each year on open software desktop publishing, data analysis and numeric and symbolic computing.

THESES

1. *Preconditioned statistical sampling techniques for* ab initio *calculations: theory and proof of principle with model calculations of defects in silicon*, Torkel Dyrbaek Engeness, Bachelor of Science in Physics, MIT, September 1996.
2. *Multiscale modeling in electronic structure calculations*, Dicle Yeşilleten, Bachelor of Science in Physics, MIT, May 1996.

3. *An investigation of the dynamics of phase transitions in Lennard-Jones fluids*, Nicolas Hadjiconstantinou, Master of Science in Physics, MIT, August 1998.

4. *Hydrolysis and Oxidation of Model Organic Compounds in Sub- and Supercritical Water: Reactor Design, Kinetics Measurements, and Modeling*, Philip A. Marrone, Doctor of Philosophy in Chemical Engineering, June 1998.
   (Co-supervised with Prof. Jefferson Tester of the Department of Chemical Engineering)

5. *Nonlinear Eigenvalue Problems*, Ross Adams Lippert, Doctor of Philosophy in Mathematics, MIT, June 1998.
   (Co-supervised with Prof. Alan Edelman of the Department of Mathematics.)

6. *SPC Solvation Energy of Methylene Chloride Reaction Complex using* Ab Initio *Charge Density*, Alok Saldanha, Bachelor of Science in Physics, MIT, May 1999.

7. *Utilizing the Density Matrix for Quantum State Extrapolation*, Kenneth P. Esler, Bachelor of Science in Physics, MIT, May 1999.

8. *Electronic Structure Theory of Dislocations in Iron*, Nichols Anthony Romero, Bachelor of Science in Physics, MIT, May 1999.

9. *Experimental and* ab initio *investigations into the fundamentals of corrosion*, in the context of supercritical water oxidation systems, Jason Alexander Cline, Doctor of Philosophy in Chemical Engineering, MIT, 2000.

10. *New perspectives on* ab initio *calculation and physical insights gained through linkage to continuum theories*, Sohrab Ismail-Beigi, Doctor of Philosophy in Physics, MIT, June 2000.

11. *New* ab initio *formulation of electron correlation and spin resonance*, Gábor Csányi, Doctor of Philosophy in Physics, MIT, September 2001.

12. *Local basis implementation for DFT++ software*, Anjali Gopalakrishnan, Master of Science in Physics, Cornell University, January 2002.

13. *Coarse-graining electronic behavior in condensed matter systems: from electrons to continuum elasticity*, Darren Eric Segall, Doctor of Philosophy in Physics, MIT, September 2002.

14. *Multiscale* ab initio *approaches to materials physics*, Torkel D. Engeness, Doctor of Philosophy in Physics, MIT, February 2003.

15. Ab initio *study of magnetic effects at material interfaces*, Dicle Yeşilleten, Doctor of Philosophy in Physics, MIT, February, 2003.

16. *New Possibilities for Securities Market Research*, Christopher Maloney, Doctor of Philosophy in Physics, Cornell University, January, 2004.

17. *Quantitative Prediction of Elastic and Anelastic Phenomena on the Nanometer Scale*, Hande Üstünel, Doctor of Philosophy in Physics, Cornell University, August, 2005.

18. *Joint Density-Functional Theory and Its Application to Systems in Solution*, Sahak A. Petrosyan, Doctor of Philosophy in Physics, Cornell University, August, 2006.

19. *Atomic level theory of the growth of crystalline oxide materials*, Daniel Ari Freedman, Doctor of Philosophy in Physics, Cornell University, Decemeber 2008.

INVITED PRESENTATIONS

1. "Precise and efficient *ab initio* molecular dynamics," Fifth International Workshop on Computational Condensed Matter Physics, Trieste, Italy, *January 1991.*

2. "Total energy calculations with a connection machine," European Research Conference on the Electronic Structure of Solids: at the Computational Leading Edge, Cambridge, United Kingdom, *September 1992.*

3. "Impurity segregation at semiconductor grain boundaries," Materials Research Society Meeting on the Theory of Materials Properties, San Francisco, California, *April 1993.*

4. "Wavelets," Fifth Annual Workshop on Recent Developments in Electronic Structure Algorithms, The Pennsylvania State University, Pennsylvania, *May 1993.*

5. "*Ab initio* study of dopant segregation at semiconductor grain boundaries," Third International Symposium on Process Modeling in Semiconductor Technology, Honolulu, Hawaii, *May 1993.*

6. "Wavelet–transform representation of the electronic structure of materials," Second Mardi Gras Conference: Toward Teraflop Computing and New Grand Challenge Applications, Baton Rouge, Louisiana, *February 1994.*

7. "*Ab initio* theory of the STM signature of impurities," Annual March Meeting of the American Physical Society, Pittsburgh, Pennsylvania, *March 1994.*

8. "Phonons: an illustrative example of the first principles calculation of an important phenomenon," Second Annual University of California — San Diego Supercomputing Center Workshop on Computational Aspects of Materials Science, San Diego, California, *July 1994.*

9. "Wavelets: an intelligent multiresolution basis for the future?" Annual Meeting of the Society of Industrial and Applied Mathematicians, San Diego, California, *July 1994.*

10. "Curvature in conjugate gradient calculations with application to materials and chemical calculations," *Proceedings of the fifth SIAM Applied Linear Algebra Conference*, ed. John G. Lewis, the Society of Industrial and Applied Mathematicians, Philadelphia (1994).

11. "Interpolets: the wavelet of the future for electronic structure calculation," Annual March Meeting of the American Physical Society, San Jose, California, *March 1995.*

12. "An interpolet basis for electronic structure calculation," Plenary talk at the Annual Physics in Computing Meeting of the American Physical Society, Pittsburgh, Pennsylvania, *June 1995.*

13. "*Ab initio* theory of electronic and mechanical structure of doped grain boundaries," Gordon Conference on Solid State Studies in Ceramics: Electrically and Chemically Active Defects, New London, New Hampshire, *July 1995.*

14. "Designer wavelets for *ab initio* electronic structure calculations," Annual Meeting of the Materials Research Society, Boston, Massachusetts, *December 1995.*

15. "Dislocation reconstruction in silicon with implications for mobility: an integrated *ab initio* – atomistic approach," University of California Institute of Theoretical Physics workshop on Modeling of Industrial Materials, Santa Barbara, California, *January 1996.*

16. "A multiscale approach to calculation of thermal averages and changes in free energy: application to reconstruction of dislocations in silicon ," University of California Institute of Theoretical Physics workshop on Modeling of Industrial Materials, Santa Barbara, California, *June 1997.*

17. "Multiscale Monte Carlo sampling for total energy electronic structure calculations," T.A. Arias, Tenth Annual Workshop on Recent Developments in Electronic Structure Algorithms, Philadelphia, Pennsylvania, *May 29-June 1, 1998.*

18. "Multiresolution analysis of electronic structure," T.A. Arias, Workshop on Wavelets and Applications in Physics and Astrophysics at the Institute for Theoretical Atomic and Molecular Physics of the Harvard-Smithsonian Center for Astrophysics, Cambridge Massachusetts, *October 8-10, 1998.*

19. "New insights into extended crystalline defects through augmenting the ab initio approach with coarse-grained levels of description," T.A. Arias, *Solid State Physics Seminar*, Oak Ridge National Laboratory, Knoxville Tennessee, *November 1998.*

20. "Semicardinal multiresolution analysis and density functional theory: exact recovery from limited samples as keystone for application of wavelets to the physical sciences," T.A. Arias, *Solid State Physics Seminar*, Vanderbilt University, Nashville Tennessee, *November 1998.*

21. "The one-body density matrix in solids: theory and practice," T.A. Arias, Ninth International Workshop on Computational Materials Science: Electronic Structure Theory & Simulations, Trieste, Italy, *January 1999.*

22. "Unraveling multiscale phenomena of defects in solids," T.A. Arias, *Physics Colloquium*, Cornell University, Ithaca, New York, *January 1999.*

23. "Beyond wavelets," *Condensed Matter Theory Seminar*, Cornell University, Ithaca, New York, *January 1999.*

24. "Multiscale science in bcc metals: reduction to practice," *Second Caltech ASCI-ASAP Center Workshop on Materials Properties*, Beckman Institute, California Institute of Technology, Pasadena, California, *February 1999.*

25. "Unraveling multiscale physics in solids," *Physics Colloquium*, University of Texas, Austin, Texas, *February 1999.*

26. "Exactness theorems for wavelets in physical calculations," *Solid State Theory Seminar*, University of Texas, Austin, Texas, *February 1999.*

27. "Beyond Wavelets: Exactness theorems for physical calculations," Annual Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics, Center for Simulational Physics, University of Georgia, Athens, Georgia, *March 1999.*

28. "Unraveling multiscale physics of defects in solids," *Physics Colloquium*, Ohio State University, Columbus, Ohio, *April 1999.*

29. "Locality of the Density Matrix in Metals, Semiconductors, and Insulators," *CECAM Workshop on Recent Developments in the Theory of Wannier Functions and other Localized Electronic Wavefunctions*, Lyon, France, *June 1999.*

30. "Density Matrix Expansions for Correlation in Many-Body Systems," *CECAM Workshop on Recent Developments in the Theory of Wannier Functions and other Localized Electronic Wavefunctions*, Lyon, France, *June 1999.*

31. "Density Matrix Extrapolation Technique for Quantum State Extrapolation," *CECAM Workshop on Recent Developments in the Theory of Wannier Functions and other Localized Electronic Wavefunctions*, Lyon, France, *June 1999.*

32. "The Science of Multiscale Modeling," *Center for Advanced Materials Research Workshop on Multiscale Modeling of Materials*, Brown University *May 2000.*

33. "New Algebraic Formulation of Density-Functional Calculation," *Third SIAM Conference on Mathematical Aspects of Materials Science (MS00)*, Philadelphia, *May 2000.*

34. "*Ab initio* study of screw dislocations in Mo and Ta: A new view of plasticity in bcc transition metals," *Dislocations 2000*, Gathersburg, Maryland, *June 2000.*

35. "Wavelet methods for solving nonlinear partial differential equations: electronic structure," *Materials Theory Across Scales,* Grenoble, France, *February 2001.*

36. "Expressive software: DFT++ algebraic formulation of *ab initio* calculations," Oak Ridge National Laboratories, Oak Ridge, Tennessee, *May 2001.*

37. "*Ab initio* theory of microscopic processes controlling mechanical response," Bodega Bay Multiscale Modeling Workshop, Bodega Bay, California, *October 2001.*

38. "Ab initio theory of plasticity," Tenth international symposium on plasticity and its current applications, Quebec City, Canada, *July 2003.*

39. "Wavelets for Robust High-Precision Calculation of the Electronic Structure of Solids," Forty-fourth Sanibel Symposium, St. Augustine, Florida, *Februrary 2004.*

40. "Predictive understanding of solvation," Multiscale modeling symposium of the International Conference on Computational and Experimental Engineering and Sciences 2004, Madeira, Portugal, *July 2004.*

41. "Toward systematic and rigorous approaches to numerical electronic structure and to continuum-atomistic coupling," *Eighth U.S. National Congress on Computational Mechanics*, Austin, Texas, *July 2005.*

REFEREED PUBLICATIONS

1. "Striated Spectral Activity in Jovian and Saturnian radio emission," by J.R. Thieman, J.K. Alexander, T.A. Arias and D.H. Staelin, *Journal of Geophysical Research* **93**:A9, 9597–9605 (September 1988).

2. "Reexamination of magnetic effects in the Bose gas," by T.A. Arias and J.D. Joannopoulos, *Physical Review* **B 39**:7, 4071–4078 (1 March 1989).

3. "The relationship between the microscopic properties of semiconducting grain boundaries and their orientation," by E. Tarnow, T.A. Arias, P.D. Bristowe, P. Dallot, G.P. Francis, J.D. Joannopoulos and M.C. Payne, in *Atomic Scale Calculations of Structure in Materials*, ed. M.S. Daw and M.A. Schluter, Materials Research Society Symposium Proceedings **193**, Pittsburgh (1990).

4. "*Ab initio* molecular dynamics techniques extended to large length–scale systems," by T.A. Arias, M.C. Payne and J.D. Joannopoulos, *Physical Review* **B 45**:5, 1538–1549 (15 January 1992).

5. "Visual revelations from silicon *ab initio* calculations," by R.H. Wolfe, M. Needels, T.A. Arias, and J.D. Joannopoulos, *IEEE Computer Graphics and Applications* **12**:4, 45–53 (July 1992).

6. "Iterative minimization techniques for *ab initio* total energy calculations: molecular dynamics and conjugate gradients," by M.C. Payne, M.P. Teter, D.C. Allan, T.A. Arias and J.D. Joannopoulos, *Reviews of Modern Physics* **64**:4, 1045–1097 (October 1992).

7. "*Ab initio* molecular dynamics: analytically continued energy functionals and insights into iterative solutions," by T.A. Arias, M.C. Payne and J.D. Joannopoulos, *Physical Review Letters* **69**:7, 1077–1080 (17 August 1992).

8. "*Ab initio* prediction of dopant segregation at elemental semiconductor grain boundaries without coordination defects," by T.A. Arias and J.D. Joannopoulos, *Physical Review Letters* **69**:23, 3330–3333 (7 December 1992).

9. "Chemical softness and impurity segregation at grain boundaries," by A. Dal Pino, Jr., M. Galván, T.A. Arias and J.D. Joannopoulos, *Journal of Chemical Physics* **98**:2, 1606–1610 (17 January 1993).

10. "Scanning–tunneling–microscopy signatures and chemical identifications of the (110) surface of Si–doped GaAs," by Jing Wang, T.A. Arias, J.D. Joannopoulos, G.W. Turner and O.L. Alerhand, *Physical Review* **B 47**:16, 10326–10334 (15 April 1993).

11. "Dimer vacancies and dimer–vacancy complexes on the Si(100) surface," by Jing Wang, T.A. Arias and J.D. Joannopoulos, *Physical Review* **B 47**:16, 10497–10508 (15 April 1993).

12. "Wavelets in electronic structure calculations," by K. Cho, T.A. Arias, J.D. Joannopoulos and Pui K. Lam, *Physical Review Letters* **71**:12, 1808–1811 (20 September 1993).

13. "Adaptive Riemannian metric for all–electron calculations," by A. Devenyi, K. Cho, T.A. Arias and J.D. Joannopoulos, *Physical Review* **B 49**:19, 13373-13376 (15 May 1994).

14. "Electron trapping and impurity segregation without defects: *ab initio* study of perfectly rebonded grain boundaries," by T.A. Arias and J.D. Joannopoulos, *Physical Review* **B 49**:7, 4525–4531 (15 February 1994).

15. "*Ab initio* theory of dislocation interactions: from close–range spontaneous annihilation to the long–range continuum limit," by T.A. Arias and J.D. Joannopoulos, *Physical Review Letters*, **73**:5, 680–683 (1 August 1994).

16. "Multiscale approach to determination of thermal properties and changes in free energy: application to reconstruction of dislocations in silicon," by T.D. Engeness and T.A. Arias, *Physical Review Letters* **79**:16, 3006–3009 (20 October 1997). Preprint: arXiv.org/abs/cond-mat/9805305 .

17. "Multiscale computation with interpolating wavelets," by Ross A. Lippert, T.A. Arias and Alan Edelman, *Journal of Computational Physics*, **140**:2, 278–310 (1 March 1998). Preprint: arXiv.org/abs/cond-mat/9805283 .

18. "Edge-driven transition in the surface structure of nanoscale silicon," by Sohrab Ismail-Beigi and T.A. Arias, *Physical Review* **B 57**:19, 11923–11926 (15 May 1998). Preprint: arXiv.org/abs/cond-mat/9805343 .

19. "Paramagnetic structure of the soliton of the 30 degrees partial dislocation in silicon," by Gàbor Csányi, Sohrab Ismail-Beigi and T.A. Arias, *Physical Review Letters* **80**:18, 3984–3987 (4 May 1998). Preprint: arXiv.org/abs/cond-mat/9805328 .

20. "Chemical Reactions and Phase Equilibria of Model Halocarbons and salts in sub- and supercritical Water (200–300 bar, 100–600 degrees C)," Jefferson W. Tester, Philip A. Marrone, Matthew M. Dipippo, Kentaro Sako, Matthew T. Reagan, Tomas Arias and William A. Peters, *Journal of Supercritical Fluids* **13**:1-3, 225–240 (1998).

21. "The geometry of algorithms with orthogonality constraints," Alan S. Edelman, Tomás A. Arias, and Steven T. Smith, *Society for Industrial and Applied Mathematics Journal on Matrix Analysis and Applications* **20**:2, 303–353 (20 October 1998). Preprint: arXiv.org/abs/physics/9806030 .

22. "Solvation effects on kinetics of methylene chloride reactions in sub- and supercritical water: theory, experiment, and *ab initio* calculations," by P.A. Marrone, T.A. Arias, W.A. Peters, and J.W. Tester, *Journal of Physical Chemistry* **A 102**:35, 7013–7028 (27 August 1998). Preprint: arXiv.org/abs/cond-mat/9807215 .

23. "Stabilizing role of itinerant ferromagnetism in intergranular cohesion in iron," by D. Yeşilleten, M. Nastar, T.A. Arias, A.T. Paxton, S. Yip, *Physical Review Letters* **81**:14, 2998–3001 (5 October 1998). Preprint: arXiv.org/abs/cond-mat/9806034 .

24. "Multiresolution analysis of electronic structure: semicardinal and wavelet bases," T.A. Arias, *Reviews of Modern Physics* **71**:1, 267–311 (January 1999). Preprint: arXiv.org/abs/cond-mat/9805262 .

25. "Locality of the density matrix in metals, semiconductors, and insulators," by Sohrab Ismail-Beigi and T.A. Arias, *Physical Review Letters* **82**:10, 2127–2130 (8 March 1999). Preprint: arXiv.org/abs/cond-mat/9805147 .

26. "Tensor–product expansions of correlation in quantum many-body systems," by Gábor Csányi, and T.A. Arias, *Physical Review* **B 61**:11, 7348–7352 (15 March 2000). Preprint: arXiv.org/abs/cond-mat/9805388 .

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