

MATERIALS RESEARCH LABORATORY, UNIVERSITY OF CALIFORNIA,  
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## Kris T. Delaney

### RESEARCH INTERESTS

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Soft condensed matter, statistical mechanics and morphology of block copolymer melts.  
Computational simulations of polymer field theories, complex-Langevin methods, coarse-graining.  
Earth-abundant alternatives to technologically relevant materials in photovoltaics and optoelectronics.  
Electronic-structure theory for computing properties of materials from first principles.  
Density functional theory, many-body perturbation theory (GW), and quantum Monte Carlo.  
Electronic, dielectric, optical, magnetic and structural properties from first principles.  
Design of novel functional materials. Multifunctional complex oxides.

### RESEARCH EXPERIENCE

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- 07/2012 - Present** Materials Research Laboratory, University of California, Santa Barbara CA, USA  
*Associate Project Scientist*
- 01/2011 - 06/2012** Materials Research Laboratory, University of California, Santa Barbara CA, USA  
*Assistant Project Scientist*
- Soft condensed matter, computational field theory for block copolymer morphology.
  - Optically and electronically active oligomers for photovoltaic applications.
  - State-of-the-art high-performance computing on graphics processing units.
- 05/2010 - 06/2010** Zernike Institute for Advanced Materials, Rijksuniversiteit Groningen Netherlands  
*ICMR International Research Fellow, visitor of Prof. Maxim Mostovoy.*
- Ferroelectric and multiferroic domain walls in uniaxial ferroelectrics.
  - Exposing topologically protected domain vortices using high-order Ginzburg-Landau theory.
- 01/2009 - 12/2010** Materials Department, University of California, Santa Barbara CA, USA  
*Associate Specialist researcher in the group of Nicola A. Spaldin.*
- Novel functional materials; multiferroics, magnetoelectrics and robust, high-*k* dielectrics.
  - Efficient methods for computing magnetoelectric responses from first principles.
  - Mapping first-principles calculations to model Hamiltonians – assessing finite-temperature field responses of materials.
- 07/2006 - 12/2008** Materials Research Laboratory, University of California, Santa Barbara CA, USA  
*Postdoctoral Scholar in the groups of Chris G. Van de Walle and Nicola A. Spaldin.*
- Optoelectronics: Efficiency losses in nitride solid-state light emitters.
  - Electronic excitations, photoemission and optical spectra from many-body methods.
  - Electronic structure of rare-earth pnictides: interdisciplinary collaboration with 7 UCSB groups.
  - Heterostructures and semiconductor/metal Schottky interfaces in polar and non-polar orientations.
- 10/2003 - 06/2006** Department of Physics, University of Illinois at Urbana-Champaign IL, USA  
*Postdoctoral Scholar in the group of David M. Ceperley and Richard M. Martin*
- Quantum Monte Carlo simulations for extended systems on highly parallel supercomputers.
  - Equilibrium phase behaviour of high-pressure hydrogen.

## EDUCATION

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- 10/2000 - 10/2003** Department of Physics, University of York York, UK  
*Doctor of Philosophy in Physics. Advisor: Prof. RW Godby*  
Awarded **K.M. Stott prize** for the best performance in a physics Ph.D.  
Thesis: Applications of Many-Body Perturbation Theory within Hedin's *GW* approximation.
- 10/1996 - 07/2000** Department of Physics, University of York York, UK  
*MPhys (Hons), Master of Physics in Theoretical Physics*  
Four-year undergraduate degree with final-year research.  
Grade: first class with honours.  
Dissertation: Diffusion of adsorbed Si atom on Si(100) surface using quantum molecular dynamics.

## TEACHING EXPERIENCE

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- July 2010** Teaching assistant for beginning graduate students at the African School on Electronic Structure Methods and Applications, Cape Town, South Africa. School also involved remote mentoring of six students on their chosen research projects for approximately one year.
- 2002-Present** Hands-on mentoring in theory, computation, presentations and writing research articles for final-year undergraduates and junior graduate students. Official mentor for three international summer research interns from 2006-2010.
- 2000-2003** Approximately 100 hours of classroom experience as primary instructor in tutorial/recitation style for beginning undergraduate students in Electromagnetism and Atomic Physics. Teaching assistant in the undergraduate computational physics laboratory.

## PUBLICATIONS

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- "Self-consistent field theory investigations of directed self-assembly in cylindrical confinement", Nabil Laachi, Tatsuhiro Iwama, [Kris T. Delaney](#), David Shykind, Robert Bristol, Corey J. Weinheimer and Glenn H. Fredrickson, **Journal of Polymer Science B: Polymer Physics** **53**, 317-326 (2015).
- "Thermodynamic and kinetic aspects of defectivity in directed self-assembly of cylinder-forming diblock copolymers in laterally confining thin channels", Bongkeun Kim, Nabil Laachi, [Kris T Delaney](#), Michael Carilli, Edward J. Kramer, and Glenn H Fredrickson, **Journal of Applied Polymer Science** **131**, 40790 (2014).
- "Improving Brush Polymer Infrared One-Dimensional Photonic Crystals via Linear Polymer Additives", Robert J Macfarlane, Bongkeun Kim, Byeongdu Lee, Raymond A Weitekamp, Christopher M Bates, Siu Fung Lee, Alice B Chang, [Kris T Delaney](#), Glenn H Fredrickson, Harry A Atwater, and Robert H Grubbs, **J. Am. Chem. Soc.** **136**, 17374 (2014).
- "A multi-species exchange model for fully fluctuating polymer field theory simulations", Dominik Duchs, [Kris T. Delaney](#), and Glenn H. Fredrickson, **J. Chem. Phys.** **141**, 174103 (2015).
- "Improving Energy Relay Dies for Dye Sensitized Solar Cells by Increasing Donor Homotransfer", Nancy D. Eisenmenger, [Kris T. Delaney](#), Venkat Ganesan, Glenn H. Fredrickson, and Michael L. Chabinyc, **J. Phys. Chem. C** **118**, 14098-14106 (2014).
- "Phase Coexistence Calculations of Reversibly Bonded Block Copolymers: A Unit Cell Gibbs Ensemble Approach", Zoltan Mester, N. A. Lynd, [Kris T. Delaney](#), and Glenn H. Fredrickson, **Macromolecules** **47**, 1865-1874 (2014).
- "Field-theoretic simulations of multi-cylinder configurations in VIA lithography", Nabil Laachi, Tatsuhiro Iwama, [Kris T. Delaney](#), David Shykind, Robert Bristol, Corey J. Weinheimer and Glenn H. Fredrickson, **Journal of Photopolymer Science and Technology** **27**, 21-24 (2014).
- "Block Copolymer Self Assembly during Rapid Solvent Evaporation: Insights into Cylinder Growth and Stability", Sean P. Paradiso, [Kris T. Delaney](#), Carlos J. García-Cervera, Hector D. Cenicerros, and Glenn H. Fredrickson, **ACS Macro Letters** **3**, 16-20 (2013).
- "Strong coupling of Jahn-Teller distortion to oxygen-octahedron rotation and functional properties in epitaxially-strained orthorhombic LaMnO<sub>3</sub>", J.-H. Lee, [Kris T. Delaney](#), Eric Bousquet, N. A. Spaldin and Karin Rabe, **Phys. Rev. B** **88**, 174426 (2013).

- “Quantification of octahedral rotations in strained LaAlO<sub>3</sub> films via synchrotron x-ray diffraction”, R. L. Johnson-Wilke, D. Marincel, S. Zhu, M. P. Warusawithana, A. Hatt, J. Sayre, [K. T. Delaney](#), R. Engel-Herbert, C. M. Schlepütz, J.-W. Kim, V. Gopalan, N. A. Spaldin, D. G. Schlom, P. J. Ryan, and S. Trolrier-McKinstry, **Phys. Rev. B** **88**, 174101 (2013).
- “The Hole Shrink Problem: Directed Self-Assembly Using Self-Consistent Field Theory”, Tatsuhiro Iwama, Nabil Laachi, [Kris T. Delaney](#), Bongkeun Kim, Su-Mi Hur, Robert Bristol, David Shykind, Corey J. Weinheimer and Glenn H. Fredrickson, **Journal of Photopolymer Science and Technology** **26**, 15-20 (2013).
- “Striped Ellipsoidal Particles by Controlled Assembly of Diblock Copolymers”, Se Gyu Jang, Debra J. Audus, Daniel Klinger, Daniel V. Krogstad, Bumjoon J. Kim, Alexandre Cameron, Sang-Woo Kim, [Kris T. Delaney](#), Su-Mi Hur, Kato L. Killops, Glenn H. Fredrickson, Edward J. Kramer and Craig J. Hawker, **J. Am. Chem. Soc.** **135**, 6649-6657 (2013).
- “Structural and Optoelectronic Characterization of RF Sputtered ZnSnN<sub>2</sub>”, Lise Lahourcade, Naomi C. Coronel, [Kris T. Delaney](#), Sujeet K. Shukla, Nicola A. Spaldin and Harry A. Atwater, **Advanced Materials** **25**, 2562-2566 (2013).
- “The hole shrink problem: Theoretical studies of directed self-assembly in cylindrical confinement”, Nabil Laachi, [Kris T. Delaney](#), Bongkeun Kim, Su-Mi Hur, Robert Bristol, David Shykind, Corey J. Weinheimer and Glenn H. Fredrickson, **Proc. SPIE 8680 - Alternative Lithographic Technologies V**, 868014 (2013).
- “Comparison of Pseudo-Spectral Algorithms for Field-Theoretic Simulations of Polymers”, Debra Audus, [Kris T. Delaney](#), Hector Cenicerros, and Glenn H. Fredrickson, **Macromolecules** **46**, 8383-8391 (2013).
- “Coherent States Formulation of Polymer Field Theory”, Xingkun Man, [Kris T. Delaney](#), Michael C. Villet, Henri Orland and Glenn H. Fredrickson, **J. Chem. Phys.** **140**, 024905 (2014).
- “Defectivity in Laterally Confined Lamella-Forming Diblock Copolymers: Thermodynamic and Kinetic Aspects”, Hassei Takahashi, Nabil Laachi, [Kris T. Delaney](#), Su-Mi Hur, Corey J. Weinheimer, David Shykind and Glenn H. Fredrickson, **Macromolecules** **45**, 6253-6265 (2012).
- “Reactivity Ratios and Mechanistic Insight for Anionic Ring-Opening Copolymerization of Epoxides”, Bongjae F. Lee, Martin Wolffs, [Kris T. Delaney](#), Johannes K. Sprafke, Frank A. Leibfarth, Craig J. Hawker and Nathaniel A. Lynd, **Macromolecules** **45**, 3722-3731 (2012).
- “Multiblock Polymers: Panacea or Pandora's Box?”, Frank S. Bates, Marc A. Hillmyer, Timothy P. Lodge, Christopher M. Bates, [Kris T. Delaney](#) and Glenn H. Fredrickson, **Science** **336**, 434-440 (2012).
- “Self-consistent field theory of directed self-assembly in laterally confined lamellae-forming diblock copolymers”, Nabil Laachi, Hassei Takahashi, [Kris T. Delaney](#), Su-Mi Hur, David Shykind, Corey J. Weinheimer and Glenn H. Fredrickson, **Proc. SPIE 8323 - Alternative Lithographic Technologies IV**, 83230K (2012).
- “Scaling Behavior and Beyond Equilibrium in the Hexagonal Manganites”, Sinead M. Griffin, Martin Lilienblum, [Kris T. Delaney](#), Yu Kumagai, Manfred Fiebig, and Nicola A. Spaldin, **Phys. Rev. X** **2**, 041022 (2012).
- “Landau theory of topological defects in multiferroic hexagonal manganites”, Sergey Artyukhin, [Kris T. Delaney](#), Nicola A. Spaldin, and Maxim Mostovoy, **Nature Materials** **13**, 42-49 (2014).
- “Polymer Field Theory Simulations on Graphics Processing Units”, [Kris T. Delaney](#) and GH Fredrickson, **Comp. Phys. Comm.** **184**, 2102-2110 (2013).
- “Anisotropic Conductance at Improper Ferroelectric Domain Walls”, D Meier, J Seidel, A Cano, [K Delaney](#), Y Kumagai, M Mostovoy, NA Spaldin, R Ramesh, and M Fiebig, **Nature Materials** **11**, 284-288 (2012).
- “Low-temperature ketene formation in materials chemistry through molecular engineering”, F Leibfarth, M Wolffs, LM Campos, [Kris T. Delaney](#), N Treat, MJ Kade, B Moon, and CJ Hawker, **Chem. Sci.** **98**, 766-771 (2012).
- “Local Density of States and Interface Effects in Semimetallic ErAs Nanoparticles Embedded in GaAs”, JK Kawasaki, R Timm, [Kris T. Delaney](#), E Lundgren, A Mikkelsen, and CJ Palmstrøm, **Phys. Rev. Lett.** **107**, 036806 (2011).
- “Indirect Auger recombination as a cause of efficiency droop in nitride light-emitting diodes”, E Kioupakis, P Rinke, [Kris T. Delaney](#), and CG Van de Walle, **Appl. Phys. Lett.** **98**, 161107 (2011).
- “Unexpectedly large electronic contribution to linear magnetoelectricity”, E Bousquet, NA Spaldin, and [Kris T. Delaney](#), **Phys. Rev. Lett.** **106**, 107202 (2011).
- “Electric and magnetic polarizabilities of hexagonal Ln<sub>2</sub>CuTiO<sub>6</sub> (Ln = Y, Dy, Ho, Er, and Yb)”, D. Choudhury, A Hazarika, A Venimadhav, C Kakarla, [Kris T. Delaney](#), P Sujatha Devi, P Mondal, R Nirmala, J Gopalakrishnan, NA Spaldin, U Waghmare, and DD Sarma, **Phys. Rev. B** **82**, 134203 (2010).
- “Microscopic theory of temperature-dependent magnetoelectric effect”, M Mostovoy, A Scaramucci, NA Spaldin, and [Kris T. Delaney](#), **Phys. Rev. Lett.** **105**, 087202 (2010).

- "Theoretical Study of Schottky-Barrier Formation at Epitaxial Rare-Earth-Metal/Semiconductor Interfaces", Kris T. Delaney, NA Spaldin, and CG Van de Walle, **Phys. Rev. B** **81**, 165312 (2010).
- "Electrical conductivity of high-pressure liquid hydrogen by quantum Monte Carlo methods", F Lin, M Morales, Kris T. Delaney, C Pierleoni, RM Martin, and DM Ceperley, **Phys. Rev. Lett.** **103**, 256401 (2009).
- "Unusual Dielectric Response in B-Site Disordered Hexagonal Transition-Metal Oxides", D Choudhury, Venimadhav, C Kakarla, Kris T. Delaney, P Sujatha Devi, Nirmala, J Gopalakrishnan, U Waghmare, NA Spaldin, and DD Sarma, **Appl. Phys. Lett.** **96**, 162903 (2010).
- "Mn<sup>3+</sup> in Trigonal Bipyramidal Coordination: a New Blue Chromophore", A Smith, H Mizoguchi, Kris T. Delaney, NA Spaldin, A Sleight, and M Subramanian, **J. Am. Chem. Soc.** **131**, 17084 (2009).
- "Auger Recombination Rates in Nitrides from First Principles", Kris T. Delaney, P Rinke, and CG Van de Walle, **Appl. Phys. Lett.** **94**, 191109 (2009).
- "Superexchange-Driven Magnetoelectricity in Magnetic Vortices", Kris T. Delaney, M Mostovoy, and NA Spaldin, **Phys. Rev. Lett.** **102**, 157203 (2009).
- "Role of Atomic Multiplets in the Electronic Structure of Rare-Earth Semiconductors and Semimetals", L Pourovskii, Kris T. Delaney, CG Van de Walle, NA Spaldin, and A Georges, **Phys. Rev. Lett.** **102**, 096401 (2009).
- "Theoretical Study of the Structural and Electronic Properties of Strained ErAs", Kris T. Delaney, NA Spaldin, and CG Van de Walle, **Phys. Rev. B** **77**, 235117 (2008).
- "Progress in Coupled Electron-Ion Monte Carlo Simulations of High-Pressure Hydrogen", C Pierleoni, Kris T. Delaney, M Morales, DM Ceperley, and M Holzmann, **Recent Prog. in Many-Body Theories** **11**, 217-232 (2008).
- "Near-infrared absorption and semimetal-semiconductor transition in 2 nm ErAs nanoparticles embedded in GaAs and AlAs", MA Scarpulla, JMO Zide, JM LeBeau, Kris T. Delaney, CG Van de Walle, and AC Gossard, **Appl. Phys. Lett.** **92**, 173116 (2008).
- "Trial Wave Functions for High-Pressure Metallic Hydrogen", C Pierleoni, Kris T. Delaney, M Morales, DM Ceperley, and M Holzmann, **Comp. Phys. Comm.** **179**, 89-97 (2008).
- "Vertex Corrections in Localized and Extended Systems", AJ Morris, M Stankovski, Kris T. Delaney, P Rinke, and RW Godby, **Phys. Rev. B** **76**, 155106 (2007).
- "Quantum Monte Carlo Simulation of the High-Pressure Molecular-Atomic Crossover in Fluid Hydrogen", Kris T. Delaney, C Pierleoni, and DM Ceperley, **Phys. Rev. Lett.** **97**, 235702 (2006).
- "Comment on 'Band-Gap Problem in Semiconductors Revisited: Effects of Core States and Many-Body Self-Consistency'", Kris Delaney, P García-González, A Rubio, P Rinke, and RW Godby, **Phys. Rev. Lett.** **93**, 249701 (2004).
- "Image States in Metal Clusters", P Rinke, Kris Delaney, P García-González, and RW Godby, **Phys. Rev. A** **70**, 063201 (2004).

Latest publication list available at <http://scholar.google.com/citations?user=vSt-CMAAAAJ&hl=en>

#### RECENT PRESENTATIONS

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|-------------------|---|
| <b>Mar. 2014</b>  | APS March Meeting, Denver, CO, USA. <ul style="list-style-type: none"> <li>▪ <i>Fluctuating Field-Theoretic Polymer Simulations of Multispecies Melts and Composites.</i></li> </ul>  |
| <b>Feb. 2014</b>  | NSF-PREM Photovoltaics Workshop, University of Texas at El Paso, TX, USA. <ul style="list-style-type: none"> <li>▪ <b>Invited:</b> <i>Introduction to Electronic Band Structures and Homo/Hetero-interfaces in Inorganic Semiconductors.</i></li> </ul> |
| <b>Feb. 2014</b>  | Complex Fluids Design Consortium Annual Meeting, Santa Barbara, CA, USA. <ul style="list-style-type: none"> <li>▪ <i>Efficient, Stable and Accurate Exchange-Based Method for FTS of Multispecies Melts.</i></li> </ul>                                 |
| <b>Sept. 2013</b> | ACS Fall Meeting, Indianapolis, IN, USA. <ul style="list-style-type: none"> <li>▪ <b>Invited:</b> <i>Progress in Fully Fluctuating Field-Theoretic Polymer Simulations.</i></li> </ul>  |
| <b>Mar. 2013</b>  | APS March Meeting, Baltimore, MD, USA. <ul style="list-style-type: none"> <li>▪ <i>Field-theory Study of Fluctuation-Induced All-Polymer Microemulsion.</i></li> </ul>  |
| <b>Feb. 2013</b>  | Complex Fluids Design Consortium Annual Meeting, Santa Barbara, CA, USA. <ul style="list-style-type: none"> <li>▪ <i>Field-theory Study of Fluctuation-Induced Microemulsion in Copolymer Blends.</i></li> </ul>  |

- Aug. 2012** ICERM Workshop, Brown University, Providence, RI, USA.  
 ■ **Invited:** *Fluctuation Phenomena in Computational Polymer Field Theory.*
- Aug. 2012** ACS Fall Meeting, Philadelphia, PA, USA.  
 ■ **Invited:** *Computational Field Theory Study of Fluctuation Induced Microemulsions in Copolymer Blends.*
- Mar. 2012** APS March Meeting, Boston, MA, USA.  
 ■ *Field-theoretic Simulations of Bicontinuous Microemulsions in Polymer Blends.*
- Jan. 2012** Materials Research Outreach Program, Santa Barbara, CA, USA.  
 ■ **Invited:** *Fully-fluctuating Field-theoretic Simulations of Co-continuous Polymer Blends.*
- Jan. 2012** Complex Fluids Design Consortium Annual Meeting, Santa Barbara, CA, USA.  
 ■ *Field-theoretic Polymer Simulations on Graphics Processing Units.*
- Mar. 2011** APS March Meeting, Dallas, TX, USA.  
 ■ *Understanding ferroelectric domain vortices in multiferroic hexagonal manganites using Ginzburg-Landau theory and first-principles methods.*
- Mar. 2010** APS March Meeting, Portland, OR, USA.  
 ■ *Efficient First-Principles Methods for Zero- and Finite-Temperature Magnetoelectric Responses.*
- Feb. 2010** Physics Colloquium, University of Denver, CO, USA.  
 ■ **Invited:** *First-Principles Techniques: How Theory Can Help Solve The Energy Problem.*
- Jan. 2010** SPIE Photonics West: Conference on LEDs, San Francisco, CA, USA.  
 ■ **Invited:** *Auger Recombination in Nitride Light Emitters: A Theoretical Perspective.*
- Mar. 2009** APS March Meeting, Pittsburgh, PA, USA.  
 ■ **Invited:** *Designing Strong Magnetoelectric Materials from First Principles.*
- Feb. 2009** Physics Colloquium, California State University, Los Angeles, CA, USA.  
 ■ **Invited:** *Functional Materials from Computational Physics.*
- Feb. 2009** Materials Research Outreach Program, Santa Barbara, CA, USA.  
 ■ **Invited:** *First-principles Studies of Semimetal/Semiconductor Interfaces.*
- Mar. 2008** APS March Meeting, New Orleans, LA, USA.  
 ■ *First-Principles Study of Large Magnetoelectric Coupling in Triangular Lattices.*
- Mar. 2007** APS March Meeting, Denver, CO, USA.  
 ■ *First-principles Studies of ErAs and ErAs/GaAs heterostructures.*
- Mar. 2006** APS March Meeting, Baltimore, MD, USA.  
 ■ *The Nature of the Hydrogen Plasma Phase Transition.*
- Jan. 2006** Materials Research Laboratory, UC Santa Barbara, CA, USA.  
 ■ **Invited:** *Understanding the Nature of Hydrogen at High Pressure from First-Principles.*
- Jan. 2006** Applied Physics Department, Yale University, New Haven, CT, USA.  
 ■ **Invited:** *A Quantum Monte Carlo Study of High-Pressure Hydrogen Fluid.*

#### PRIZES AND SCHOLARSHIPS

- May 2010** ICMR International Research Fellowship for six-week collaboration at Zernike Institute for Advanced Materials, Rijksuniversiteit Groningen.
- Sept. 2005** MCC Award to attend the Psi-k 2005 conference.
- Jul. 2004** K.M. Stott Prize awarded for the best Ph.D. thesis; one awarded per year in Physics.
- Mar. 2003** UK Institute of Physics Barber Trust Fellowship to attend the March Meeting of the American Physical Society.
- Apr. 2002** Electronic Structure Symposium Poster Prize at the IOP CMMP/EPS 2002 conference.

## PROFESSIONAL ACTIVITIES

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- 2010-Present** Peer reviewer of research proposals submitted to the US Department of Energy.
- 2007-Present** Direct mentor for CISEI summer research interns.
- 2003-Present** Referee for Phys. Rev. Lett., Phys. Rev. B, J. Chem. Phys., J. Phys.: Cond. Mat. and New J. Phys.
- 2001-2003** Editor of the York Department of Physics newsletter.
- 2001-2002** Student Representative on the graduate students' Board of Studies in the Department of Physics, University of York.
- 1997-1998** University of York Physics Society Treasurer.

## REFERENCES

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| Prof. Glenn H. Fredrickson<br><br>Materials Research Lab.<br>University of California,<br>Santa Barbara, CA<br>93106-5050, USA<br><br>Tel. +1 (805) 893-8308<br>Email: <a href="mailto:ghf@mrl.ucsb.edu">ghf@mrl.ucsb.edu</a>            | Prof. Dr. Nicola Spaldin<br><br>ETH Zurich<br>Materials Theory (D-MATL)<br>HIT E 43.3 - 42.1<br>Wolfgang-Pauli-Strasse 27<br>CH-8093 Zürich, Switzerland<br><br>Tel. +41 44 633 37 55<br>Email: <a href="mailto:nicola.spaldin@mat.ethz.ch">nicola.spaldin@mat.ethz.ch</a> | Prof. Richard M. Martin<br><br>Department of Physics,<br>University of Illinois,<br>1110 W. Green St.,<br>Urbana, IL 61801, USA<br><br>Tel. +1 (217) 333-4229<br>Email: <a href="mailto:rmartin@uiuc.edu">rmartin@uiuc.edu</a>             |
| Prof. David M. Ceperley<br><br>Department of Physics,<br>University of Illinois,<br>1110 W. Green St.,<br>Urbana, IL 61801, USA<br><br>Tel. +1 (217) 244-0646<br>Email: <a href="mailto:ceperley@illinois.edu">ceperley@illinois.edu</a> | Prof. Rex W. Godby<br><br>Department of Physics,<br>University of York,<br>Heslington,<br>York YO10 5DD, UK<br><br>Tel. +44 (0)1904 432231<br>Email: <a href="mailto:rwg3@york.ac.uk">rwg3@york.ac.uk</a>  | Prof. Chris G. Van de Walle<br><br>Materials Department,<br>University of California,<br>Santa Barbara, CA<br>93106-5050, USA<br><br>Tel. +1 (805) 893-7144<br>Email: <a href="mailto:vandewalle@mrl.ucsb.edu">vandewalle@mrl.ucsb.edu</a> |