

Elif Ertekin

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PROFESSIONAL PREPARATION

B.S. in Engineering Science and Mechanics, Penn State University	1999
B.S. in Mathematics, Penn State University	1999
M.S. in Engineering Science, Penn State University	2000
M.S. in Materials Science and Engineering, University of California, Berkeley	2003
Ph.D. in Materials Science and Engineering, University of California, Berkeley	2006

RESEARCH APPOINTMENTS

- Assistant Professor, Dept. of Mechanical Science & Engineering, UIUC 2011-present
- Assistant Professor, Materials Research Laboratory, UIUC 2011-present
- Post-doctoral Associate, Dept. of Materials Science & Engineering, MIT 2009-2011
Advisor: Prof. Jeffrey C. Grossman
- Post-doctoral Associate, Berkeley Nanoscience and Nanoengineering Institute, UCB 2007-2009
Advisor: Prof. Jeffrey C. Grossman and Prof. Daryl C. Chrzan
- Graduate Research Fellow & Research Assistant, 2000-2006
Dept. of Materials Science & Engineering, UCB
Advisor: Prof. Daryl C. Chrzan
- Research Intern, Intelligent Micromachines Division, Sandia National Labs 2000

SCIENTIFIC HIGHLIGHTS

- authored/co-authored 20 peer-reviewed journal publications
- delivered over 50 oral presentations at technical conferences and university/academic seminars
- ~520 citations according to ISI Web of Science, H-index = 10

RESEARCH INTERESTS

Computational modeling; simulation of fundamental materials processes; atomic-scale materials design; and collaboration with experiment to address real-world challenges including

- Energy & Environment
 - design of new materials for advanced photovoltaics
 - hybrid systems and interface design for photocatalytic water splitting
 - nanostructuring for thermoelectrics
- Thermal transport in nanostructured materials
 - Coupled phonon-strain interactions, defects in low-dimensional systems
- Optics, Electronics, and Opto-electronics
 - wide band gap oxides for low power electronics
 - functional interfaces for complex oxides
- Computational Modeling and Simulation framework development
 - High accuracy method development for modeling of point defects in solids, quantum Monte Carlo
 - Modeling growth and synthesis

ACADEMIC HONORS AND AWARDS

Materials Research Society Best Poster Award, 2006, 2012

Intel Corporation Graduate Fellowship, 2005

National Science Foundation Graduate Fellowship, 2001-2003

Pennsylvania State University, University Scholar, 1996-2000

Xerox Undergraduate Research Award & Fenlon Undergraduate Thesis Award, 2000

Teaching Awards:

Outstanding Graduate Student Instructor Award, 2004

Teachers Ranked as Excellent by their Students, Fall 2011, Fall 2012, Spring 2013, Fall 2013, Fall 2014.

PROFESSIONAL ACTIVITIES AND COMMUNITY OUTREACH

- Organizer, 2013 E-MRS annual meeting “Materials for Photocatalysis and Photoelectrochemistry” symposium
- Manuscript Reviewer: Physical Review Letters, Physical Review B, Journal of Electronic Materials, European Physical Journal B, Nano Letters, Thin Solid Films, Extreme Mechanics Letters, and others; Review Editor for Frontiers in Materials.
- International Advisory Committee, International Conference on Defects in Semiconductors (2013-date)
- Member, Materials Research Society, American Physical Society, ASM International, American Chemical Society, The Minerals, Metals, and Materials Society
- Proposal Reviewer/Panelist: National Science Foundation, US Dept. of Energy
- Nanohub Course Tools: Developer of simulation tools and course material for the NSF-sponsored nanoHUB project at <http://www.nanohub.org>.
- Curriculum development, Introduced and developed a new special topics course entitled “Fundamentals of Modern Photovoltaics” into the Mechanical Science & Engineering curriculum, Fall 2011. Website: <http://ertekin.mechse.illinois.edu/fteaching/fundpv>
- Workshops and Other Outreach:
 - 2011 - Workshop on Synergy with and Learning from Nature (NSF, ESF, and Tubitak), Istanbul
 - 2007 - Workshop on Predictive Modeling of Nanomaterial Properties, Session Co-Chair, D.C.
 - 2012-2014 - Hands-on Photovoltaics Experience, PV summer school at NREL.
 - 2014 – Illinois Computational Science and Engineering, ICME Workshop
- Mechanical Science and Engineering, U Illinois Departmental Service:
 - Department Seminar Committee, 2011-present, MechSE UIUC
 - Building Renovation Committee, 2012-present, MechSE UIUC
 - Strategic Instructional Initiatives Program, 2012-present, MechSE UIUC
 - Undergraduate Programs Committee, 2012-present, MechSE UIUC
 - Co-Director, 2013-2015, Girls Building Awesome Machines summer camp for high school girls
 - MechSE Advisory Board, 2013-2015
 - Photovoltaics Exhibit Organizer, MechSE Open House and Engineering Open House, 2011-2015

PUBLICATIONS

Refereed Journal Articles:

1. D. Nandwana, E. Ertekin. “Ripples, strain, and misfit dislocations: structure of graphene - boron nitride superlattice interfaces”, *Nano Lett.* (2015). DOI: 10.1021/nl505005t
2. S. Ida, N. Kim, E. Ertekin, S. Takenaka, T. Ishihara. “Photocatalytic Reaction Centers in Two-Dimensional Titanium Oxide Crystals”. *J. Am. Chem. Soc.* **137** 239–244 (2015). DOI: 10.1021/ja509970z
3. S. Lee, A.R. Damodaran, P. Gorai, N. Oh, J.A. Moyer, J.-H. Kwon, N. Ferdous, A. Shah, Z. Chen, E. Breckenfeld, R.V.K. Mangalam, P.V. Braun, P. Schiffer, M. Shim, J.-M. Zuo, E. Ertekin and L.W. Martin. “A novel, layered phase in Ti-rich SrTiO₃ epitaxial thin films”, *Advanced Materials* **27** 861 (2015). DOI: 10.1002/adma.201403602
4. T. Zhu, E. Ertekin, “Phonon transport on two-dimensional graphene/boron nitride superlattices”, *Phys.*

Rev. B **90** 195209 (2014). DOI: 10.1103/PhysRevB.90.195209

5. B. K. Newman, E. Ertekin, J. T. Sullivan, M. T. Winkler, M. A. Marcus, S. C. Fakra, M.-J. Sher, E. Mazur, J. C. Grossman, T. Buonassisi. "Extended X-ray absorption fine structure spectroscopy of selenium-hyperdoped silicon", *J. Appl. Phys.* **114**, 133507 (2013).
6. E. Ertekin, L. K. Wagner, and J. C. Grossman. "Point-defect optical transitions and thermal ionization energies from quantum Monte Carlo methods: application to the F-center defect in MgO", *Physical Review B* **87** 155210 (2013).
7. E. Ertekin, V. Srinivasan, J. Ravichandran, P. Rossen, W. Siemons, A. Majumdar, R. Ramesh, and J. C. Grossman. "Interplay between intrinsic defects, doping, and free carrier concentration in SrTiO₃ thin films", *Phys. Rev. B* **85** 195460 (2012).
8. E. Ertekin, M. T. Winkler, D. Recht, A. J. Said, M. J. Aziz, T. Buonassisi, and J. C. Grossman. "Insulator-to-metal transition in selenium-hyperdoped silicon: observation and origin", *Phys. Rev. Lett.* **108** 026401 (2012).
9. D. Schebarchov, S. C. Hendy, E. Ertekin, and J. C. Grossman. "Interplay of wetting and elasticity in the nucleation of carbon nanotubes", *Phys. Rev. Lett.* **107** 185503 (2011).
10. S. Chen, E. Ertekin, D. C. Chrzan. "Plasticity in carbon nanotubes: cooperative conservative dislocation motion", *Phys. Rev. B* **81** 155417 (2010).
11. E. Ertekin, M.S. Daw, D.C. Chrzan. "Topological description of the Stone-Wales defect formation energy in graphene and carbon nanotubes", *Phys. Rev. B* **79** 155421 (2009).
12. J. Cao, E. Ertekin, V. Srinivasan, S. Huang, W. Fan, H. Zheng, J. W. L. Yim, D. R. Khanal, D. F. Ogletree, J. C. Grossman, J. Wu. "Strain engineering and one-dimensional organization of metal insulator domains in single crystal VO₂ beams", *Nat. Nanotechnol.* **4** 732 (2009).
13. W. Fan, S. Huang, J. Cao, E. Ertekin, C. Barrett, D. R. Khanal, J. C. Grossman, J. Wu. "Superelastic metal-insulator phase transition in single-crystal VO₂ nanobeams", *Phys. Rev. B Rapid Commun.* **80** 241105(R) (2009).
14. G. E. Begtrup, W. Gannett, J. C. Meyer, T. D. Yuzvinsky, B.M. Kessler, E. Ertekin, J. C. Grossman, A. Zettl. "Facets of nanotube synthesis: high-resolution electron microscopy study and density functional theory calculations", *Phys. Rev. B* **79** 205409 (2009).
15. E. Ertekin, M.S. Daw, D.C. Chrzan. "Elasticity theory of topological defects in carbon nanotubes and graphene", *Phil. Mag. Lett.* **88** 159 (2008).
16. E. Ertekin, D.C. Chrzan. "Ideal torsional strengths and stiffnesses of carbon nanotubes", *Phys. Rev. B* **72** 45425 (2005).
17. E. Ertekin, P.A. Greaney, D.C. Chrzan, T.D. Sands. "Equilibrium limits of coherency in strained nanowire heterostructures", *J. Appl. Phys.* **97** 114325 (2005).
18. E. Ertekin, A. Lakhtakia. "Optical interconnects realizable with thin-film helicoidal bianisotropic mediums", *Proc. R. Soc. Lon. Ser-A* **457** 817 (2001).
19. E. Ertekin, V.C. Venugopal, A. Lakhtakia. "Effect of substrate and lid on the optical response of an axially excited slab of a dielectric thin-film helicoidal bianisotropic medium", *Microw. Opt. Techn. Lett.* **20** 218 (1999).
20. E. Ertekin, A. Lakhtakia. "Sculptured thin film Solc filters for optical sensing of gas concentration", *Eur. Phys. J. - Appl. Phys.* **5** 45 (1999).

Work Submitted for Publication:

1. T. Zhu, E. Ertekin. "Anomalous strain effects on transitional phonon flow in graphene, boron nitride and graphene/boron nitride superlattices", submitted (2015).
2. D. Nandwana, E. Ertekin. "Lattice mismatch induced rippling behavior of graphene – boron nitride superlattices", submitted (2015).
3. P. Gorai, E. G. Seebauer, E. Ertekin. "Density functional theory analysis of adsorption of molecular oxygen on polar and non-polar zinc oxide surfaces", submitted (2014).

Conference Proceedings:

1. E. Ertekin, P.A. Greaney, T.D. Sands, and D.C. Chrzan. "Equilibrium analysis of lattice-mismatched nanowire heterostructures", *J. Mater. Res.* 737 769 (2003).
2. J. Seo, E. Ertekin, M.S. Pio, L.P. Lee. [Conference Paper] "Self-assembly templates by selective plasma surface modification of micropatterned photoresist", *Proc. IEEE MEMS* 2002 192 (2002).
3. A. Lakhtakia, P. D. Sunal, V. C. Venugopal, E. Ertekin. "Homogenization and optical response properties of sculptured thin films", *Proc. SPIE Conf.*, 3790 77 (1999).
4. V.C. Venugopal, A. Lakhtakia, E. Ertekin. "Optical and electronic applications of sculptured thin films", *Proc. SPIE Conf.*, 3790 195 (1999).

PRESENTATIONS

Invited Presentations:

1. Psi-K 2015 Conference, Title TBD, San Sebastian, Spain 2015.
2. CECAM (Centre Européen de Calcul Atomique et Moléculaire) - Workshop on Stochastic Wavefunction Methods in Quantum Chemistry, Electronic Structure Theory and Condensed Matter Physics, "Quantum Monte Carlo methods as a tool for design of real engineering materials," Lausanne, Switzerland, April 2015.
3. Nothing is perfect: the quantum mechanics of defects, "A random walk through point defect electronic structure: insights from quantum Monte Carlo," Ascona Switzerland, April 2015.
4. National Renewable Energy Laboratory, "Challenging methods for high-accuracy modeling of challenging materials," Materials Sciences Division Seminar, Golden CO, February 2015.
5. (Keynote speaker), 5th International Symposium on Transparent Conductive Materials, "What we can learn from many-body descriptions of doping and defects in oxides," Chania, Crete, October 2014.
6. Argonne National Laboratories, "Quantum Monte Carlo Methods: Applications to Semiconductor Bulk and Defect Properties," Materials Science Division Seminar, Argonne IL, August 2014.
7. International Conference on Hydrogen Production 2014, "Ultra-thin polarizable TiO₂/BaTiO₃ heterostructures for dynamically controllable surface chemistry: first-principles study," Kyushu University, Japan, February 2014.
8. TMS 2014 Annual Meeting and Exhibition, "Statistical approach to modeling the defect-mediated plasticity and deformation of low-dimensional nanostructures," San Diego, February 2014.
9. CECAM-Workshop on Functional Oxides for Emerging Technologies, "Interplay between polarity, surface chemistry in oxide materials" Bremen, Germany, Oct 2013.
10. CECAM-Workshop on Nanophonics, "Graphene-Boron Nitride Superlattices for Nanoscale Heat Transport" Bremen, Germany, Aug 2013.
11. International Conference on Defects in Semiconductors, "High Accuracy Modeling of Point Defects in Semiconductors via quantum Monte Carlo methods", Bologna, Italy, to be held July 2013.
12. Institute for Condensed Matter Theory, Department of Physics, University of Illinois, April 2013.
13. Workshop on Accelerating the Development of Earth-Abundant Photovoltaics, March 2013.
14. Johns Hopkins University, Department of Materials Science & Engineering, "Atomic Scale Materials Design for Photovoltaics and Photocatalysis". Baltimore, MD, to be held Nov 2012.
15. Arçelik Corporation, "Photovoltaics: Technologies, Markets, Trends, and Future Projections". Istanbul Turkey, June 2012.
16. University of Utah, Department of Materials Science & Engineering. "Predictive and Guided Materials Design-by-Computation: Application to Optical Properties, Advanced Photovoltaics, and Photocatalysis". Salt Lake City UT, Apr 2012.
17. University of Illinois, Energy and Sustainability Engineering Seminar Series. "Photovoltaics: Trends, Technologies, Prospects". Urbana IL, Apr 2012.
18. Iowa State University, Department of Materials Science & Engineering. "Predicting Structure–Property Relationships Across Length Scales: From Nanoscale Plasticity to Advanced Photovoltaics". Ames IA, Nov

2011.

19. University of Illinois, Department of Mechanical Science & Engineering, Materials Interest Group. "Multiscale approach to dislocation dynamics in carbon nanotubes and graphene". Urbana IL, Oct 2011.
20. University of Colorado at Boulder, Department of Mechanical Engineering. "Understanding, Predicting, and Designing the Properties of Advanced Materials". Boulder CO, Feb 2011.
21. University of Illinois, Department of Mechanical Science & Engineering. "Understanding, Predicting, and Designing the Properties of Advanced Materials". Urbana, IL, Dec 2010.
22. University of Southern California, Department of Mechanical Engineering. "Modeling mechanisms of deformation and plasticity in graphene and carbon nanotubes". Los Angeles, CA, April 2008.
23. National Science Foundation Symposium of Multi-Scale Dislocation Dynamics. "Towards dislocation dynamics in carbon nanotubes and graphene". University of California at San Diego, La Jolla CA, Jan 2008.
24. Clemson University, Department of Astronomy & Physics and Department of Mechanical Engineering Joint Colloquium. "Defects in Carbon Nanotubes: Implications for Mechanical Properties." Clemson SC, April 2006.