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Contents

1 Education

1.1 My Education

- B.S., 1996, NATIONAL UNIVERSITY OF MEXICO, Physics.
- M.S., 2000, MASSACHUSETTS INSTITUTE OF TECHNOLOGY, Materials Science and Engineering.
- Ph.D., 2003, MASSACHUSETTS INSTITUTE OF TECHNOLOGY, Materials Science and Engineering with a minor in Applied Mathematics.

1.2 Thesis

- B.S. *"Automated Signal Detection System for the Bicolor Birefringence Technique."*
- M.S. *"A Mathematical Model of the Physical Vapor Deposition of Thermal Barrier Coatings."*
- Ph.D. *"Modeling Effects of Microstructure for Electrically Active Materials."*

1.3 Professional Employment

- August 2015 - present. Professor, School of Materials Engineering, Purdue University, West Lafayette, IN.
- August, 2011 - 2015. Associate Professor, School of Materials Engineering, Purdue University, West Lafayette, IN.
- August, 2005 - July, 2011. Assistant Professor, School of Materials Engineering, Purdue University, West Lafayette, IN.
- 2003 - August, 2005. Postdoctoral position, National Institute of Standards and Technology, Gaithersburg, Maryland. Developed public domain computational tools to understand the relations between material properties, crystal structure, and microstructure.
- January, 2000 - January, 2003 Research Assistant, Massachusetts Institute of Technology, Cambridge, MA.
- September, 1999 - December, 1999. Teaching Assistant, Massachusetts Institute of Technology, Cambridge, MA. 3.091. *Introduction to Solid State Chemistry*. Undergraduate introductory course to Chemistry, Materials Science, and generalities of solid state phase transformations.

1.4 Professional Societies

- American Ceramics Society (ACerS)
- The Electrochemical Society (ECS).
- The Materials Research Society (MRS).
- The Minerals, Metals, and Materials Society (TMS).
- Interpore: International Society for Porous Media

2 Research

2.1 Summary

2.1.1 Introduction

The focus lies on the development of fundamental materials science as the necessary basis to engineer the underlying physical and microstructural properties in emerging materials and devices. Developed materials science theories and numerical models establish correlations that link atomistic, mesocontinuum, and macroscopic scales and quantify the impact of individual chemistries on the macroscopic response, reliability, and time-dependent performance of emerging material applications. Example contributions are shown below.

2.1.2 The Materials Science and Design of Rechargeable Batteries

The effort has contributed to the fundamental and applied understanding of battery technology, such as the effect of electrode morphologies, crystallographic anisotropy, and the mesoscale porous microstructure, on the macroscopic power density and reliability. The research pioneered the development of fundamental science to rationalize the effect of tortuosity and area density, critical to control power density (*e.g.*, see Section 2.2, items 33, 38, 39, 41, 50). The effort has resulted on scientific publications which detail the effect of porous microstructures on battery performance (*e.g.*, see Section 2.2, items 4, 12, 19, 24, 30), predict advantages and disadvantages of high power densities and out-of-the box designs (*e.g.*, see Section 2.2, items 12, 40), to detail the interfacial and crystallographic anisotropy interactions during multiple charge/discharge cycles (*e.g.*, see Section 2.2, items 24, 30). Long standing technological challenges such as lithium dendrite formation are being tackled in an effort to maximize the performance of batteries for electric vehicles to understand the role of microstructural defects, including the architecture of separators, on lithium dendrite growth (*e.g.*, see Section 2.2, items 35, 47, 49, 57).

2.1.3 Design of Lead-Free Piezoelectric Materials

The effort has contributed to identify the underlying mechanisms that control the ferroelectric domains-grain boundaries interactions for bulk ceramics (*e.g.*, see Section 2.2, items 5, 6, 9, 18, 32). The effects of size in ferroelectric materials for thin film applications have been analyzed to establish fabrication maps where tailored switching behavior can be tuned to generate high performance or low power FeRAMs (*e.g.*, see Section 2.2, items 21, 26, 45). In addition, the optimal piezoelectric behavior of lead-free materials, such as BT, BNKT and BNT, are being identified (*e.g.*, see Section 2.2, items 34, 52,63). The developed theoretical methodologies use experimental EBSD sections to reconstruct, numerically verify, and experimentally engineer improved materials that are readily fabricated in the laboratory (*e.g.*, see Section 2.2, items 31, 52).

2.1.4 (In,Ga)N-Based Light-Emission Technologies

In complete departure from traditional approaches to generate light for residential and commercial applications, materials science and engineering criteria was developed to improve the efficacy of (In,Ga)N based Light Emission Technologies. Real-time visualization approaches (2.2.27), dislocation-free conditions (2.2.20 and 22), improved mechanical reliability (2.2.24), and zero built-in electrical field conditions (2.2.28) have been identified to contribute to reach the 2020 DOE goal of improved lighting technology.

2.1.5 Basic Science and Microstructural Evolution of Materials

A generalized theoretical framework is being developed to predict the microstructure evolution that results from the applied processing parameters. Applications include: 1) the processing of pharmaceutical materials (2.2.48), its mechanical reliability (2.2.36, 37, 43, 46, 53), and its dissolution kinetics (2.2.42). 2) the Physical Vapor Deposition of single component polycrystalline thin film growth, where physical mechanisms such as evaporation and condensation, the Gibbs-Thomson effect, line-of-sight, and grain impingement and rotation have been incorporated to concurrently describe thin film evolution (2.2.29 and 44). And 3) the Electric-field assisted sintering of ionic ceramics, where the conditions and mechanisms that control the incubation and dynamics of the flash event, as well as the grain growth coarsening kinetics after flash are identified.

2.1.6 Equilibrium Properties and Kinetics of Charged Surfaces and Interfaces

By starting from fundamental principles, a comprehensive space-charge treatment consistent with the laws of thermodynamics and Maxwell's equations is being established (2.2.3). The generalized theory naturally includes the free energy contributions and the multiphysical interactions in the vicinity of grain boundaries, surfaces, and interfaces(2.2.47). Weak and strong dilution limits are described to predict the appearance of experimentally observed interfaces (2.2.58), and their phase transitions (2.2.2). We demonstrate the validity of this theory for polycrystalline materials for energy-related applications. This is the first type of modeling approach where the grain boundary core naturally includes electrochemical and chemomechanical effects (2.2.58).

2.2 Refereed Journal Papers

Year: 2019 | 2017-18 | 2016 | 2014 | 2012 | 2010 | 2008-

– **2004**

1. *"Real-Time, High-Gain, Computer Controlled Amplifier for Optical Detection Systems."* R. E. García, J. Hernandez-Cordero, and E. Geffroy. *Review of Scientific Instruments*, Vol. 73, number 1, pgs 203-208. January 2002.

2. *"Effect of Charge Separation on the Stability of Large Wavelength Fluctuations During Spinodal Decomposition."* C. M. Bishop, R. E. García, and W. C. Carter. *Acta Materialia*, (51) 1517-1524, 2003.

3. *"Thermodynamically Consistent Variational Principles with Applications to Electrically and Magnetically Active Systems."* R. E. García, C. M. Bishop, and W. C. Carter. *Acta Materialia*, (52) 11-21, 2004.

2005

4. *"Microstructural Modeling and Design of Rechargeable Lithium-Ion Batteries."* R. E. García, Y.-Ming Chiang, W. C. Carter, P. Limthongkul, and C. M. Bishop. *The Journal of the Electrochemical Society.* (152) 1, A255-A263, 2005.

5. *"The Effect of Texture and Microstructure on the Macroscopic Properties of Polycrystalline Piezoelectrics: Application to $BaTiO_3$ and PZN-PT."* R. E. García, W. C. Carter, and S. A. Langer. *Journal of the American Ceramics Society*, 88 [3] 750-757 (2005).

6. *"Finite Element Implementation of a Thermodynamic Description of Piezoelectric Microstructures."* R. E. García, W. C. Carter, and S. A. Langer. *Journal of the American Ceramics Society*, 88 [3] 742-749 (2005).

2006

7. *"Challenges and Results for Quantitative Piezoelectric Hysteresis Measurements."* B. D. Huey, R. Nath, R. E. García, and J. E. Blendell Microscopy and Microanalysis 11, 6, (2006).

8. *"Ionic Colloidal Crystals: Ordered, Multicomponent Structures via Controlled Heterocoagulation."* G. R. Maskaly, R. E. García, W. C. Carter, and Y.-M. Chiang. *Physical Review* E. 011402 (2006).

9. *"Virtual Piezo-Force Microscopy of Polycrystalline Ferroelectric Films."* R. E. García, B. Huey, and J. E. Blendell. *The Journal of Applied Physics* 100, 064105 (2006).

2007

10. *"Influence of Grain Boundaries and Texture on Ferroelectric Domain Hysteresis."* B. Huey, R. E. Garcia, J. E. Blendell and R. Nath. *Journal of Minerals, Metals and Materials Society*, 59 [1] 17, 2007.

11. *"Correlations Between Crystallographic Texture and Grain Boundary Character in Polycrystalline Materials."* R. E. García, and M. D. *Vaudin Acta Materialia*, (55) 5728-5735, 2007.

12. *"Spatially-Resolved Modeling of Microstructurally Complex Battery Architectures."* R. E. García, and Y.-M. Chiang. *Journal of the Electrochemical Society* (154) A856-A864, 2007.

2008

13. *"Image-Based Finite Element Mesh Construction for Material Microstructures."* A. C. E. Reid, S. A. Langer*, R. C. Lua, V. R. Coffman, S.-I. Haan*, and R. E. García*. *Computational Materials Science* (43) 989-999, 2008.

2009

14. *"Modeling Microstructures in OOF2."* A. C. E. Reid, R. C. Lua, R. E. García, V. Coffman, and S. A. Langer. *International Journal of the Materials and Product Technology.* Vol. 35 3/4, pp. 361-373 (2009).

15. "Optimizing the Microstructure in Polycrystalline Ferroelectrics for Random Access Memory Applications." H. A. Murdoch and R. E. García *International Journal of the Materials and Product Technology.* Vol. 35 Nos. 3/4, pp. 293-310 (2009).

16. *"Application of a High Throughput Bioluminescence-based Method and Mathematical Model for the Quantitative Comparison of Polymer Microbicide Efficiency."* T. R. Stratton, R. E. García, B. M. Applegate, and J. P. Youngblood. *Biomacromolecules*, 10 (5), pp. 1173-1180 (2009).

17. *"Microstructural Modeling of Ferroelectric Materials: State of the Art, Challenges and Opportunities."* S. Leach and R. E. García. *Materials Science Forum* (606) 119-134, 2009.

18. *"Domain Switching Mechanisms in Polycrystalline Ferroelectrics with Asymmetric Hysteretic Behavior."* E. Anton, R. E. García, J. Blendell, T. Key, and K. Bowman. *The Journal of Applied Physics.* 105 024107 (2009).

19. *"The Effect of Microstructure on the Galvanostatic Discharge of Graphite Anode Electrodes in $LiCoO_2$-Based Rocking-Chair Rechargeable Batteries."* M. C. Smith, R. E. García, and Q. C. Horn. *The Journal of the Electrochemical Society.* (156) A896-A904, 2009.

2010

20. *"Dislocation Filtering in GaN Nanostructures."* R. Colby, Z. Liang, I. Wildeson, T. D. Sands, R. E. García and E. A. Stach. *Nano Letters*, 10(5) 1568-73, 2010.

21. *"Collective Dynamics in Nanostructured Polycrystalline Ferroelectric Thin Films Using Local Time-Resolved Measurements and Switching Spectroscopy"* S. Wicks, K. Seal, S. Jesse, V. Anbusathaiah, S. Leach, R. E. García, S. V. Kalinin, V. Nagarajan. *Acta Materialia*, (58) pp. 67-75, 2010.

22. *"GaN Nanostructure Design for Optimal Dislocation Filtering"* Z. Liang, R. Colby, I. Wildeson, T. D. Sands, E. A. Stach, and R. E. García., *The Journal of Applied Physics.* 108, 074313 (2010).

23. *"Gibbs: Symbolic Computation of Thermodynamic Properties and Phase Equilibria."* T. Cool, A. Bartol, M. Kasenga, K. Modi, and R. E. García. *Computer Coupling of Phase Diagram and Thermochemistry.* 34 (2010) 393404.

24. *"Nanoscale Mapping of ion Diffusion in a Lithium-ion Battery Cathode."* N. Balke, S. Jesse, A.N. Morozovska, E. Eliseev, D.W. Chung, Y. Kim, L. Adamczyk, R.E. García, N. Dudney, and S.V. Kalinin. *Nature Nanotechnology*, 5(10):749-754.

25. *"III-Nitride Nanopyramid LEDs Grown by Organometallic Vapor Phase Epitaxy."* I. H. Wildeson, R. Colby, D. A. Ewoldt, Z. Liang, D. N. Zakharov, N. J. Zaluzec, R. E. García, E. A. Stach, and T. D. Sands. *The Journal of Applied Physics.* 108, 074313 (2010).

2011

26. *"Edge and Finite Size Effects in Polycrystalline Ferroelectrics."* S. Leach, R. E. García, and V. Nagarajan. *Acta Materialia.* 59, 191-201. (2011).

27. *"Augmenting Heteronanostructure Visualization with Haptic Feedback."* M. Abdul-Massih, B. Benes, T. Zhang, C. Platzer, W. Leavenworth, H. Zhuo, R. E. García, and Z. Liang. Advances in Visual Computing 6939, 627-636, (2011).

28. *"Built-in Electric Field Minimization in (In, Ga)N Nanoheterostructures."* Z. Liang, I. H. Wildeson, R. Colby, D. A. Ewoldt, T. Zhang, T. D. Sands, E. A. Stach, B. Benes, and R. E. García. Nano Letters (11) 4515-4519, (2011).

29. *"Kinetics of Congruent Vaporization of ZnO Islands."* B. J. Kim, R. E. García, and E. A. Stach Phys. Rev. Lett. (107) 146101, (2011).

30. *"Virtual Electrochemical Strain Microscopy of Polycrystalline $LiCoO_2$ Films."* D.-W. Chung, N. Balke, S. V. Kalinin, and R. E. García*. Journal of the Electrochemical Society (158) A1083-A1089, (2011).

2012

31. *"Ferroelastic Domains and Anisotropy in Lead Free Piezoelectrics."* B. Z. Li, C. Fancher, J. E. Blendell, R. E. García, K. J. Bowman. Materials Science Forum (702) 995-998, 2012.

32. "*Modeling 180° Domain Switching Population Dynamics in Polycrystalline Ferroelectrics.*" Z. Zhao, C. Fancher, K. Bowman, and R. E. García. Journal of the American Ceramics Society. 95 [5] 1619-1627 (2012).

33. *"An Analytical Method to Determine Tortuosity in Rechargeable Battery Electrodes."* B. Vijayaraghavan, D. Ely, Y.-M. Chiang, R. García-García, and R. E. García. The Journal of the Electrochemical Society,159 (5) A548-A552 (2012).).

2013

34. *"Microstructure Design of Lead-Free Piezoelectric Ceramics."* S. Lee, T. Key, S. Wang, Z. Liang, R. E. García, G. Rohrer, and T. Tani. Journal of the European Ceramic Society. 33 (2) 313-326 (2013).

35. *"Heterogeneous Nucleation and Growth of Lithium Electrodeposits on Negative Electrodes."* D. R. Ely and R. E. García. The Journal of the Electrochemical Society. 160(4): A662-A668, 2013.

36. *"Stochastic Failure of Isotropic Brittle Materials with Uniform Porosity."* O. Keles, R. E. García, and K. Bowman. Acta Materialia 61 (8):2853-2862, (2013).

37. *"Deviations from Weibull Statistics in Brittle Porous Materials."* O. Keles, R. E. García, and K. Bowman. Acta Materialia**.** 61(19): 7207-7215, 2013.

38. *"Validity of the Bruggeman Relation for Porous Electrodes."* D.-W. Chung, M. Ebner, D. R. Ely, V. Wood, and R. E. García. Modelling and Simulation in Materials Science and Engineering 21 (7), 074009, 2013.

2014

39. *"Tortuosity Anisotropy in Lithium-Ion Battery Electrodes."* M. Ebner, D.-W. Chung, R. E. García, and V. Wood Advanced Energy Materials. 4(5): 1301278, 2014.

40. *"Designing 3D Conical-Shaped Lithium-Ion Microelectrodes."* D.G. Lim, D.-W. Chung, R. Kohler, J. Proell, C. Scherr, W. Pfleging, R. E. García*. The Journal of the Electrochemical Society. 161(3): A302-A307, 2014.

41. *"Particle Size Polydispersity in Li-Ion Batteries."* D.-W. Chung, P.R. Shearing, N.P. Brandon, S.J. Harris, R.E. García* The Journal of the Electrochemical Society. 161(3):A422-A430, 2014.

42. *"Ostwald-Freundlich Diffusion-Limited Dissolution Kinetics of Nanoparticles."* D. R. Ely*, R. E. García, M. Thomes Powder Technology. 257, 120-123, 2014.

43. *"Pore-crack orientation effects on fracture behavior of brittle porous materials."* O. Keles, R. E. García, and K. Bowman. International Journal of Fracture. 187(2):293-299, 2014.

44. *"From Process to Modules: End-to-End Modeling of CSS-Deposited CdTe Solar Cells."* E.S. Mungan, Y. Wang, S. Dongaonkar, D.R. Ely, R.E. García, and M.A. Alam IEEE Journal of Photovoltaics. 4(3): 954-961, 2014.

45. *"Correlated inter-grain switching in polycrystalline ferroelectric thin films."* Y. Jing, S. Leach, J.E. Blendell*, and R. E. García* Journal of Applied Physics. 116(12):124102, 2014.

46. *"Failure variability in porous glasses: Stress interactions, crack orientation, and crack size."* O. Keles, R. E. García, and K. Bowman. Journal of the American Ceramics Society. 97: 3967-3972, 2014.

47. *"Phase Field Kinetics of Lithium Electrodeposits."* D. R. Ely, A. Jana, and R. E. García*. Journal of Power Sources. 272:581-594, 2014.

48. *"Spheronization Process Particle Kinematics Determine by Discrete Element Simulations and Particle Image Velocimetry Measurements."* M. Koster, M. Thomes, and R. E. García. International Journal of Pharmaceutics. 477(1):81-87, 2014.

2015

49. *"Dendrite-Separator Interactions in Lithium-Based Batteries."* A. Jana, D. R. Ely, and R. E. García*. Journal of Power Sources. 275:912-921, 2015.

2016

50. "*Microstructural Effects on the Average Properties in Porous Battery Electrodes.*" R. García- García and R. E. García*. Journal of Power Sources. (309):11-19, 2016.

51. "*Gibbs Computational Simulation as a teaching tool for Students' Understanding of Thermodynamics of Materials Concepts.*" O. Alabi, A.J. Magana, and R.E. García Journal of Materials Education, 37:239-259, 2016.

2017-2018

52. "*Kinetically stabilized metastable polarization states in ferroelectric ceramics.*" Z. Zhao, Y. Cao, R.E. García. Journal of the European Ceramic Society. 37(2), 573-581, 2017.

53. *"Sensitivity of Fracture Strength in Porous Glass."* O. Keles, R. E. García, and K. Bowman. Journal of Applied Glass Science, 8(1):116-123, 2017.

54. "*Physically-based Reduced-Order Capacity Loss Model for Graphite Anodes in Li-Ion Battery Cells.*" X. Jin, A. Vora, V. Hoshing, G. Shaver, T. Saha, R.E. García, O. Wasynczuk, S. Varigonda. Journal of Power Sources. 342:750-761, 2017.

55. "*The role of ceramic and glass science research in meeting societal challenges: Report from an NSF-sponsored workshop.*" K.T. Faber, T. Asefa, M. Backhaus-Ricoult, R. Brow, J.Y. Chan, S. Dillon, W.G Fahrenholtz, M.W. Finnis, J.E. Garay, R.E. García, Y. Gogotsi, S.M. Haile, J. Halloran, J. Hu, L. Huang, S.D. Jacobsen, E. Lara-Curzio, J. LeBeau, W.E. Lee, C.G. Levi, I. Levin, J.A. Lewis, D.M. Lipkin, K. Lu, J. Luo, J.-P. Maria, L.W. Martin, S. Martin, G. Messing, A. Navrotsky, N.P. Padture, C. Randall, G.S. Rohrer, A. Rosenflanz, T.A. Schaedler, D.G. Schlom, A. Sehirlioglu,

A.J. Stevenson, T. Tani, V. Tikare, S. Trolier-McKinstry, H. Wang, B. Yildiz. Journal of the American Ceramic Society. 100(5):1777-1803, 2017.

56. "*Writing In-Code Comments to Self-Explain in Computational Science and Engineering Education.*" C. Vieira, M. Falk, R.E. García, and A. Magana ACM Transactions on Computing Education. 17:80-85, 2017.

57. "*Lithium Dendrite Growth Mechanisms in Liquid Electrolytes.*" A. Jana, R.E. García. Nano Energy. 41:552-565, 2017.

58. "*Charged Interfaces: Electrochemical and Mechanical Effects.*" V. Karra, W. Chueh, R.E. García. **Energy & Environmental Science.** 11:1993-2000, 2018.

59. "*Integrating Computational Science Tools into a Thermodynamic Course.*" C. Vieira, A. Jana, M. Konieczny, R.E. García, and A. Magana. **Journal of Science Education and Technology.** January 2018. link.

60. "*High temperature deformability of ductile flash sintered ceramics via in-situ compression.*", J. Cho, Q. Li , H. Wang, Z. Fan, J. Li, S. Xue, S. Karra, H. Wang, T.B. Holland, A.K. Mukherjee, R.E. García, X. Zhang. **Nature Communications.** 9 (1): 2063, 2018.

2019

61. *"The effects of external fields in ceramic sintering."* SK Jha, XL Phuah, J Luo, CP Grigoropoulos, H Wang, E García, B. Reeja-Jayan. **Journal of the American Ceramics Society.** 102(1):5-31, 2019. link

62. *"Key microstructural characteristics in flash sintered 3YSZ critical for enhanced sintering process."* H Wang, XL Phuah, J Li, TB Holland, KSN Vikrant, L Qiang, CS Hellberg, N Bernstein, RE García, A Mukherjee, X Zhang, H Wang. **Ceramics International.** 45:1251-1257, 2019. link

63. "*Phase Coexistence Near the Morphotropic Phase Boundary.*" OA Torres-Matheus, RE García, CM Bishop. **Acta Materialia.** 164:577-585, 2019. link

64. "*Charged Grain Boundary Transitions in Ionic Ceramics for Energy Applications.*" V. Karra*, R.E. García. **npj Computational Materials.** 5:24, 2019. link

65. "*Physical, On the Fly, Capacity Degradation Prediction of $LiNiMnCoO_2$-Graphite Cells.*" A. Jana*, G. M. Shaver, and R.E. García. **Journal of Power Sources.** 422:185–195, 2019 link

2.3 Refereed Conference or Symposium Publications

1. *"Computational Materials Science and Engineering Education: A Survey of Trends and Needs."* K. Thornton,* S. Nola,* R.E. García,* M. Asta,* and G. B. Olson, *Journal of Metals*, October 2009.

2. *"Modeling and Optimization of Polymer-Based Bulk Heterojunction (BH) Solar Cells."* B. Ray,* P.R. Nair, and R. E. García, and M. Alam, International Electron Devices Meeting (IEDM), In Proceedings, Baltimore, MD, December, 2009.

3. *"FiPy and OOF: Computational Simulation as Learning Tools to Convey Concepts and Ideas of Modeling and Simulation of Computational Materials."* A. Magana,* R. E. García. American Society for Engineering Education Annual Conference. In Proceedings, Louisville, KY, 9 pages, June 20-23, 2010.

4. *"Work in Progress: Exploring Student Representational Approaches in Solving Rechargeable Battery Design Problems."* O. Ogunwuyi*, A. Magaña, and R. E. García. IEEE Frontiers in Education Conference. Oklahoma City, OK. October 23-26. In Proceedings, 2013.

5. *"Exploring Student Computational Practices in Solving Complex Engineering Design Problems."* O. Alabi*, A. Magaña, and R. E. García. Proceedings of the 121th ASEE Annual Conference and Exposition. Indianapolis, IN. June, 2014. In Proceedings, 2014.

6. *"In-code Comments as Self-explanation Strategy."* C. Vieira*, A. Jana, A. Magana, and R. E. García. SIGSE, Memphis, TN . March 2-5th, 2016.

7. *"An Exploratory Study of the Role of Modeling and Simulation in Supporting or Hindering Engineering Students' Problem Solving Skills."* U.A. Shaikh*, C. Vieira, A. Magana, and R. E. García. 122nd ASEE Annual Conference & Exposition. Seattle, WA, June 14-17, 2015.

8. *"Interactive Computer Aided Design of Electrochemical Systems."* L. D. Robinson*, A. Jana*, R. E. García. The Summer Undergraduate Research Fellowship (SURF) Symposium 10 August 2015. Purdue University, West Lafayette, Indiana, USA.

9. "*Physically-based Reduced-Order Capacity Loss Model for Graphite Anodes in Li-Ion Battery Cells.*" X. Jin*, A. Vora, V. Hoshing, G. Shaver, T. Saha, R.E. García, O. Wasynczuk, S. Varigonda. American Control Conference (ACC), 80-85, 2017.

2.4 Books and Book Chapters

1. *"Microstructural Modeling of Multifunctional Material Properties: The OOF Project."* R. E. García, A. C. E. Reid, S. A. Langer, and W. C. Carter. Invited chapter in **"Continuum Scale Simulation of Engineering Materials."** Dierk Raabe, Franz

Roters, Frédéric Barlat, Long-Qing Chen (eds.), Wiley-VCH, Weinheim (2005). ISBN 3-527-30760-5.

2. *"Developments in Strategic Materials"* H.-T.Lin, K. Koumoto, W. M. Kriven, R. E. García, I. E. Reimanis, and D. P. Norton (eds.) J. Wiley & Sons (2009), New Jersey. ISBN 978-0-470-34500-9.

2.5 Software

1. Object Oriented Finite Element Analysis for Materials Science Software (OOF). S. A. Langer, A. C. E. Reid, R. E. García, V. Coffman, S.-I. Haan, R. Lua. (2003 -) Description: OOF is a public domain scientific software aimed to study the effects of microstructure on the properties of materials. The software combines advanced image analysis and finite element methods, and provides a user-friendly interface. (2,347 nanoHUB users, 40,117 runs) http://www.ctcms.nist.gov/oof/

2. Virtual Kinetics of Materials Laboratory (VKML). A. Bartol,* M. J. Waters,* M. McLennan, and R. E. García. (2007 -). Description: VKML is a cloud-computing program to study the kinetics of materials. This software provides an easy-to-use graphical user interface to deploy microstructural evolution models, such as dendrite and grain growth, impingement, and coarsening of materials.

https://www.nanohub.org/tools/vkmllive/ (Web-Based Scientific Script Editor, 1,153 nanoHUB users, 13,167 runs).

https://www.nanohub.org/tools/vkmlggs/ (Dendritic Growth, 371 nanoHUB users, 2,051 runs)

https://www.nanohub.org/tools/vkmlpsgg/ (Polycrystalline Growth and Coarsening, 442 nanoHUB users, 2,102 runs)

https://www.nanohub.org/tools/vkmlsd/(Spinodal Decomposition, 523 nanoHUB users, 6,778 runs)

https://www.nanohub.org/tools/vkmlsd3d/ (Spinodal Decomposition 3D, 368 nanoHUB users, 1,072 runs)

3. VKMLgui. A. Bartol,* M. McLennan, and R. E. García. (2009-). Description: VKMLgui is a python-based set of libraries to deploy graphical user interfaces for scientific applications. The aim of the libraries is to remove the barrier to develop scientific applications with customizable GUIs. The focus has been VKML-Live, FiPy, Gibbs, and Gibbs-Live. (1,153 nanoHUB users, 13,167 runs) https://www.nanohub.org/tools/vkmllive/

4. Gibbs: Symbolic Computation of Thermodynamic Properties and Phase Equilibria T. Cool,* A. Bartol, M. Kasenga, K. Modi, and R. E. García. (2008 -) Description: Gibbs is a general purpose open source, python-based framework to perform multiphysical equilibrium calculations of material properties. The developed architecture allows to prototype symbolic and numerical representations of materials by starting from analytic models or tabulated experimental data. These constructions are based on the addition of arbitrary energy contributions that range from the traditional thermochemical, mechanical, to surface tension

contributions. Gibbs seamlessly interfaces with FiPy to prototype interdiffusion and microstructural evolution (phase field) models. Through its flexible Graphical User Interface, Gibbs allows rapid deployment of computational thermodynamic applications with intuitive interfaces, and through the developed viewers direct visualization and analysis of data can be readily performed for those physical properties that are relevant for the problem at hand. (460 nanoHUB users, 3,209 runs) http://nanohub.org/tools/gibbs

5. Gibbs-Live. T. Cool* and R. E. García. (2009 -) Description: Gibbs-Live is a cloud computing application that provides a web interface to Gibbs. This online implementation of the application provides a default set of examples that exemplify all the basic capabilities of Gibbs and allows the user to freely upload, edit, deploy, save results and edit programs. Gibbs-Live is based on VKML-Live, a web environment to develop microstructural evolution models by using FiPy. Here, a text editor allows to user to articulate Python-based symbolic models and use them to simulate the thermodynamic equilibrium or as a starting point to model phase field applications. The developed web interface completely removes the barrier of installing the code, and is currently used in supporting Purdue University's MSE 260 Thermodynamics of Materials, where students develop physical intuition, scientific knowledge, and analyze trends in thermodynamic problems. (460 nanoHUB users, 3,209 runs) http://nanohub.org/tools/gibbs

6. FiPy-Based Simulation Modules for Learning the Kinetics of Materials. R. E. García. (2007 - 2008). Description: Series of lectures to learn modeling and simulation of materials through the use of FiPy. Each module is accompanied by a set of slides (in PowerPoint, KeyNote, and QuickTime formats), and two or more representative simulation programs. https://www.matforge.org/fipy/wiki/FiPyExamples

7. Piezos3D: Three-Dimensional Modeling of Piezoelectric Microstructures. S. Lee,* Z. Liang* and R. E. García. (2010-). Description: Simulation software to predict three-dimensional properties of piezoelectric materials of arbitrary topologies. Program uses experimentally-determined Electron Back Scattered Diffraction Patterns to reconstruct the three-dimensional material phases, grains, pores, and crystallographic orientation of each material feature to simulate the electrical, mechanical, and electromechanical properties of emerging material microstructures. Program is currently closed source.

8. Batts3D: Three-Dimensional Modeling of Battery Microstructures. B. Vijayaraghavan, D.-W. Chung, R.E. García. (2012-). Description: Simulation software to predict three-dimensional properties of battery electrode materials of arbitrary topologies. Program uses computer-generated, experimentally-determined Electron Back Scattered Diffraction Patterns, and CT scans to reconstruct the three-dimensional material phases, grains, pores, and crystallographic orientation of each material feature to simulate the electrical, mechanical, and electrochemical properties of emerging battery electrode microstructures. Program is currently closed source.

9. kMC: kinetic Monte Carlo Simulations of Materials. D. Ely and R.E. García. (2013-). Description: kMC is a set of scientific libraries designed to deploy kinetic Monte Carlo simulations. kMC allows the user to intuitively generate crystal lattices to simulate, post process, and visualize the kinetic Monte Carlo-based atomistic evolution of materials. Philo-

sophically, kMC was designed to directly interface with any kinetic Monte Carlo application and to provide a uniform, user friendly interface to rapidly deploy advanced simulations. Organizationally, kMC is a virtual portal to couple and integrate multiple length scales computational materials science applications, such as OOF, FiPy, etc. Specifically, kMC provides a very flexible Python application programming interface (API) that allows to rapidly program complex atomistic simulations, while simultaneously taking advantage of the speed of the C++ core infrastructure. https://nanohub.org/tools/kmc/ (currently closed)

10. Equilibrium Wulff Shape Generator. R. E. García and J. E. Blendell. (2012 -). Online version of Wulffman, an open source software developed by Andrew Roosen, Ryan McCormack, and W. Craig Carter. Wulffman is a program for interactively examining the Wulff shapes of crystals with specified symmetries. https://nanohub.org/tools/wulffman/ (947 nanoHUB users, 7,730 runs)

11. Dualfoil.py: Porous Electrochemistry for Rechargeable Batteries. L. Robinson and R. E. García (2015 -) Online, GUI-enabled version of the widely popular dualfoil (aka, Newman model), and open source software aimed to simulate the time-dependent response of battery materials. Dualfoil.py is a flexible application programming interface that allows for hierarchical control over the dualfoil legacy code (Newman model) and visualization modules, and provides the user with the ability to rapidly set up complex, multiscale simulations. By making use of the object-oriented nature of Python, dualfoil.py allows the user to generate, organize, and visualize the electrochemical responses from various rechargeable battery systems. This versatile program allows for users of any skill level to achieve robust results in a control oriented and easily deployable manner. https://nanohub.org/tools/dualfoil/ (292 nanoHUB users, 3,528 runs).

2.6 Other Publications

1. *"The OOF2 Manual."* Stephen A Langer, Andrew CE Reid, SI Haan, RE García, RC Lua, VR Coffman. NIST, Gaithersburg, MD, USA, 2008.

2. *"Response surface measurement for BiFeO3-CoFe2O4 multiferroic nanocomposite."* BE Piccione*, JE Blendell, RE García. Applications of Ferroelectrics, 2008. ISAF 2008. 17th IEEE International Symposium on the. (2):1-3, 2008.

3. *"Publisher's Note:"GaN nanostructure design for optimal dislocation filtering"[J. Appl. Phys. 108, 074313 (2010)]"* Zhiwen Liang*, Robert Colby*, Isaac H Wildeson, David A Ewoldt, Timothy D Sands, Eric A Stach, R Edwin García. Journal of Applied Physics 108(10):9901.

4. *"Python-based Simulation Tool for Kinetic Monte Carlo."* Zaiwei Zhang*, R Edwin García. (October 18, 2013). The Summer Undergraduate Research Fellowship (SURF). Paper 7.

   http://docs.lib.purdue.edu/surf/2013/presentations/7

5. *"Kinetic Monte Carlo Simulations."* Jingyuan Liang*, R. Edwin García, Ding-Wen Tony Chung, David Ely. The Summer Undergraduate Research Fellowship (SURF). Paper 56 (2014).

   http://docs.lib.purdue.edu/surf/2013/presentations/56

6. *"Computation of Piezo-electric Materials."* Seung Yun Song* and R Edwin García. The Summer Undergraduate Research Fellowship (SURF). Paper 34.

   http://docs.lib.purdue.edu/surf/2013/presentations/34

7. *"Simulation of Bio-Inspired Porous Battery Electrodes."* R. Gupta, R. Tu, and R. E. García Undergraduate Research Fellowship (SURF). Paper 50 (2014).

   http://docs.lib.purdue.edu/surf/2014/presentations/50/

8. *"Simulation of Bio-Inspired Porous Battery Separators."* Y. Xie, A. Jana, and R. E. García Undergraduate Research Fellowship (SURF). Paper 130 (2014).

   http://docs.lib.purdue.edu/surf/2014/presentations/130/

9. *"Corrigendum to "Deviations from Weibull Statistics in Brittle Porous Materials"[Acta Mater. 61 (2013) 7207-7215]"* O. Keles, R. E. García, and K. J. Bowman. Acta Materialia, 68: 339-340, 2014.

10. *"Corrigendum to "Stochastic failure of isotropic, brittle materials with uniform porosity"[Acta Mater. 61 (2013) 2853-2862]"* O. Keles, R. E. García, and K. J. Bowman. Acta Materialia, 68: 341-342, 2014.

11. *"Interactive Computer Aided Design of Electrochemical Systems."* L. Robinson A. Jana, and R. E. García Undergraduate Research Fellowship (SURF). Paper 1 (2015). http://docs.lib.purdue.edu/surf/2015/presentations/1/

2.7 Contributed Conference Presentations

1. (Poster)"The Effect of Microstructure on the Macroscopic Properties of Polycrystalline Piezoelectrics." R. E. García*, W. C. Carter, and S. A. Langer. Materials Research Society Meeting. Boston, MA, November, 1998.

2. "The Effect of Microstructure on the Macroscopic Properties of Polycrystalline Ferroelectrics." R. E. García*, W. C. Carter, and S. A. Langer. American Physics Society, Computational Physics Division. Cambridge, MA, July, 2000.

3. (Poster)"The Effect of Microstructure on the Macroscopic Properties of Polycrystalline Piezoelectrics." R. E. García*, W. C. Carter, and S. A. Langer. Materials Research Society, National Meeting. Boston, MA, November, 1999.

4. "The Effect of Microstructure on the Macroscopic Properties of Polycrystalline Ferroelectrics." R. E. García*, W. C. Carter, S. A. Langer and E. R. Fuller. American Ceramics Society, Electronics Division. Clemson, University, South Carolina, October, 2000.

2.7 Contributed Conference Presentations

5. "The Effect of texture on the Macroscopic Properties of Polycrystalline Ferroelectrics." R. E. García*, W. C. Carter and S. A. Langer. Materials Research Society Meeting, Boston, MA, November, 2000.

6. "Investigation of the Magnitude of the Chemical Driving Force Required to Form Space Charge Nanodomains in Relaxor Ferroelectrics." C.M. Bishop*, R.E. García, A.N. Soukhojak, W.C. Carter, and Y.-M. Chiang, Symposium AA, Materials Research Society Meeting, Boston, MA, November, 2000.

7. "The Effect of Texture on the Macroscopic Properties of Polycrystalline Ferroelectrics." R. E. García*, W. C. Carter, and S. A. Langer. American Ceramic Society Annual Meeting, Indianapolis, IN, April, 2001.

8. "The Effect of Texture on the Macroscopic Properties of Polycrystalline Ferroelectrics." R. E. García*, W. C. Carter, and S. A. Langer. NIST, Gaithersburg, MD, April, 2001.

9. (Poster)"The Effect of Texture on the Macroscopic Properties of Polycrystalline Ferroelectrics." R. E. García*, W. C. Carter, and S. A. Langer. Solid State Studies in Ceramics, Gordon Research Conference, New Hampshire, August, 2001.

10. (Poster)"The Effect of Texture on the Macroscopic Properties of Polycrystalline Ferroelectrics." R. E. García*, W. C. Carter, and S. A. Langer. Materials Research Society Meeting, Boston, MA, November, 2001.

11. "The Effect of Microstructure on the Performance of Electroactive Devices." R. E. García*, W. C. Carter, and S. A. Langer. Singapore-MIT Alliance Annual Meeting, Singapore, January, 2002.

12. "Incorporating Electromagnetic Effects in Variational Formulations of Materials Processes." R. E. García*, C. M. Bishop, and W. C. Carter. NIST, Gaithersburg, MD, March 2002.

13. "Microstructural Design in Rechargeable Lithium-Ion Batteries." R. E. García*, C. M. Bishop, P. Limthongkul, W. C. Carter, S. A. Langer, and Y.-M. Chiang. American Ceramics Society Annual Meeting, St. Louis, MO, April, 2002.

14. "The Effect of Crystallographic Texture on Piezoelectric Ceramics." R. E. García*, W. C. Carter, and S. A. Langer. American Ceramics Society Annual Meeting, St. Louis, MO, April, 2002.

15. (Poster)"The Effect of Crystallographic Texture on Piezoelectric Ceramics." R. E. García*, W. C. Carter and S. A. Langer. Solid State Studies in Ceramics, Gordon Research Conference, New Hampshire, August 2002.

16. "Microstructural Design in Rechargeable Lithium-Ion Batteries." R. E. García*, C. M. Bishop, P. Limthongkul, W. C. Carter, S. A. Langer, and Y.-M. Chiang. Solid State Studies in Ceramics, Gordon Research Conference, New Hampshire, August, 2002.

17. "Microstructural Design of Rechargeable Lithium-Ion Batteries." R. E. García*, C. M. Bishop, P. Limthongkul, W. C. Carter, S. A. Langer, and Y.-M. Chiang. Fall Meeting of the Electrochemical Society, Orlando, Florida. October, 2003.

18. (Poster)"Microstructural Design in Rechargeable Lithium-Ion Batteries." R. E. García*, C. M. Bishop, P. Limthongkul, W. C. Carter, S. A. Langer, and Y.-M. Chiang. Solid State Studies in Ceramics, Gordon Research Conference, New Hampshire, August, 2003.

2.7 Contributed Conference Presentations

19. "Microstructural Design of Rechargeable Lithium-Ion Batteries." R. E. García*, C. M. Bishop, P. Limthongkul, W. C. Carter, S. A. Langer, and Y.-M. Chiang. 106th Annual Meeting and Exposition of the American Ceramics Society. Indianapolis, Indiana. April 18-21, 2004.

20. "Microstructural Modeling and Design of Multifunctional Ceramics." R. E. García*, W. C. Carter, Y.-M. Chiang, S. A. Langer, C. Bishop, P. Limthongkul, and M. Vaudin. 56th Pacific Coast Regional and Basic Science Division, Washington, Seattle, September, 2004.

21. "Microstructural Modeling and Design of Rechargeable Lithium-Ion Batteries." R. E. García*, W. C. Carter, and Y.-M. Chiang. Fall Meeting of the Electrochemical Society, Honolulu, Hawaii, October, 2004.

22. "The Effect of Microstructure on the Domain Stability of Polycrystalline Ferroelectric PZT Films." R. E. García*, J. E. Blendell, and B. Huey. Annual Meeting of the American Ceramics Society, Baltimore, Maryland. April, 2005.

23. "The Effect of Microstructure on the Domain Stability of Polycrystalline Ferroelectric PZT Films." R. E. García*, J. E. Blendell, and B. Huey. PacRIM Meeting of the American Ceramics Society, Maui, Hawaii, September, 2005.

24. "Microstructural Modeling and Design of Advanced Three-Dimensional Rechargeable Lithium-Ion Batteries." R. E. García*, and Y.-M. Chiang. Fall Meeting of the Electrochemical Society, Los Angeles, California. October, 2005.

25. "Texture and Microstructure Design of Electrochemical Actuators." R. Edwin García*, and Yet-Ming Chiang. Fall Meeting of the Electrochemical Society, Los Angeles, California. October, 2005.

26. "Microstructural Optimization Rechargeable Lithium-Ion Batteries." R. E. García*, and Y.-M. Chiang. Fall Meeting of the Materials Research Society, Boston, Massachusetts. December, 2005.

27. "The Effect of Microstructure on the Performance of Electrochemical Actuators." R. E. García*, and Y.-M. Chiang. Fall Meeting of the Materials Research Society, Boston, Massachusetts. December, 2005.

28. "Microstructure Modeling of Thermoelectric Nanowire Composites Generators" M. J. Howell*, R. E. García, T. Sands. Fall Meeting of the Materials Research Society, Boston, Massachusetts. November, 2006.

29. "Microstructural Design of Solid Oxide Fuel Cells" K. E. Yamamoto*, R. E. García. Fall Meeting of the Materials Research Society, Boston, Massachusetts. November, 2006.

30. "Microstructural Design of Rechargeable Lithium-Ion Batteries for High Power Density Applications." R. E. García* and Y.-M. Chiang. Fall Meeting of the Materials Research Society, Boston, Massachusetts, November, 2006.

31. "Modeling and Design of Microstructurally Complex Rechargeable Lithium-In Batteries." R. E. García* and Y.-M. Chiang. Spring Meeting of the Electrochemical Society, Chicago, Illinois. May, 2007.

32. "Introduction to the Object Oriented Finite Element Modeling of Material Microstructures." ECE Department, the nanoHUB, Purdue University. R. E. García*. June, 2007.

2.7 Contributed Conference Presentations

33. (Poster) "Engineering the Thermoelectric Behavior in Nanodots, Nanowires, and Polycrystalline Materials." M. J. Howell*, R. E. García, T. Sands. Solid State Studies in Ceramics, Gordon Research Conference, August 2007.

34. (Poster) "2D and 3D Design of InGaN Nanostructures for White Light Emitting Diodes." Z. Liang,* R. E. García. Solid State Studies in Ceramics, Gordon Research Conference, August 2007.

35. "Engineering the Thermoelectric Behavior in Nanodots, Nanowires, and Polycrystalline Materials." M. J. Howell, R. E. García*, T. Sands. Materials Science and Technology 2007 Conference Exhibition, Detroit, Michigan. October, 2007.

36. "Strain Engineering if InGaN-based LEDs through Numerical Modeling." Z. Liang and R. E. García*. Materials Science and Technology 2007 Conference Exhibition, Detroit, Michigan, October, 2007.

37. "Tailoring the Ragone Plot through Microstructure Design." R. E. García and Y.-M. Chiang. Fall Meeting of the Electrochemical Society, Washington, DC, October, 2007.

38. "The Effect of Microstructure on the Switching of Polycrystalline Ferroelectrics." E. Anton, R. E. García*, J. Blendell, and K. Bowman . American Ceramic Society, Daytona Beach, Florida, January, 2008.

39. "InGaN-Based Nanostructures for High-Performance Light Emitting Diodes" R. E. García*. American Ceramic Society, Daytona Beach, Florida, January, 2008.

40. "The Effect of Microstructure on the Local and Macroscopic Switching of Polycrystalline Ferroelectric Films." R. E. García*. The Minerals, Mining and Materials Society, New Orleans, March, 2008.

41. "Microstructure Modeling and Design of Solid Oxide Fuel Cells." K. Yamamoto and R. E. García*. The Minerals, Mining and Materials Society, New Orleans, March 2008.

42. "The Effect of Crystallographic Texture on Ferroelectric Ceramics." R. E. García*. International Conference on Texture Materials. Pittsburgh, PA, June, 2008.

43. "The Effect of Microstructure in Thermoelectric Nanodots, Nanowire Composites, and Polycrystalline Materials." R. E. García. International Conference on Texture Materials, Pittsburgh, PA, June, 2008.

44. "The Effect of Microstructure on the Ferroelectric Switching of Polycrystalline Films." R. E. García*, E. Anton, J. Blendell, and K. Bowman, Materials Science & Technology Conference and Exhibition, October 2008.

45. "Microstructure Design of Solid Oxide Fuel Cells." K. Yamamoto, R. E. García*. Materials Science & Technology Conference and Exhibition, October, 2008.

46. "FiPy Round Table: Applications to Research and Education." R. E. García*. The Minerals, Mining and Materials Society, San Francisco, California, February 16, 2009. (partial financial support)

47. "Public Domain Simulation Tools for the Kinetics and Thermodynamics of Materials Education." R. E. García*, M. Waters, and M. Kasenga. The Minerals, Mining and Materials Society, San Francisco, California, February 16, 2009.

48. "Status of Computational Materials Education in the US: Recent Results and Surveys." M. Asta,* K. Thornton, R. E. García. The Minerals, Mining and Materials Society,

San Francisco, California, February 16, 2009.

49. "Grain Boundaries-Ferroelectric Domain Interactions in Polycrystalline Ferroelectrics." R. E. García*, S. Leach, C. Fancher, J. Blendell and K. Bowman. The Minerals, Mining and Materials Society, San Francisco, California, February 18, 2009.

50. "Microstructure Design of Solid Oxide Fuel Cells." K. Yamamoto, R. E. García*. The Minerals, Mining and Materials Society, San Francisco, California, February 18, 2009.

51. "Gibbs Round Table: Vision, Concept, and Architecture." R. E. García*. The Minerals, Mining and Materials Society, San Francisco, California, February 19, 2009.

52. "Modeling and Design of Dislocation-Free Nanostructured InGaN-Based Light Emittig Devices." Z. Liang, R. E. García*, R. Colby, E. A. Stach, I. Wildeson, D. Ewoldt, D. Zakharov, J. L. Schroeder, and T. Sands. Materials Research Society, San Francisco, April 14, 2009.

53. "InGaAlN Nanorod LEDs for Green Electroluminescence." I. Wildeson*, D. Ewoldt, R. Colby, Z. Liang, D. Zakharov, R. E. García, E. A. Stach, and T. Sands. Materials Research Society, San Francisco, April 14, 2009.

54. "Microstructure Design of Portable Power Sources through Finite Element Analysis." M. Smith and R. E. García.* Materials Research Society, San Francisco, April 15, 2009.

55. "Characterization of InGaN Nanorod-based LEDs by Transmission Electron Microscopy." R. Colby*, D. Zakharov, I. Wildeson, D. Ewoldt, Z. Liang, R. E. García, E. A. Stach, and T. Sands. Materials Research Society, San Francisco, April 15, 2009.

56. "Grain Boundaries-Ferroelectric Domains Interactions in Polycrystalline Ferroelectrics." S. Leach and R. E. García*. Materials Research Society, San Francisco, April 17, 2009.'

57. "Microstructure Design of Solid Oxide Fuel Cells." K. Yamamoto and R. E. García*. Vancouver, Canada, American Ceramic Society PacRim Meeting 09, June 2, 2009.

58. "Grain Boundaries-Ferroelectric Domains Interactions in Polycrystalline Ceramics." Z. Zhao, C. Fancher, T. Cool, and R. E. García*. Vancouver, Canada, American Ceramic Society PacRim Meeting 09, June 3, 2009. (partial financial support

59. (Poster) "Modeling Switching Mechanisms in Bipolar, Sesquipolar, and Unipolar Loaded Polycrystalline Ferroelectric Ceramics." Z. Zao, R. E. García, K. Bowman*, and J. Blendell, International Symposium on Applications of Ferroelectrics meeting, Xian, China, August, 2009.

60. "Modeling and Design of Dislocation-Free InGaN-Based Nanostructures for Light Emitting Diodes." Z. Liang, R. Colby, R. E. García*, D. Zakharov, I. Wildeson, E. Stach, and T. Sands, Materials Science and Technology, Pittsburgh, PA, October 27, 2009.

61. "Three-Dimensional Modeling of Piezoelectric Microstructures." S. Lee, T. Key, G. Rohrer, T. Tani, and R. E. García*. Materials Science and Technology, Sosman Symposium, Pittsburgh, PA, October 28, 2009.

62. "Modeling Switching Mechanisms in Bipolar, Sesquipolar, and Unipolar Loaded Polycrystalline Ferroelectric Ceramics." Z. Zhao, K. Bowman, J. Blendell, and R. E. García*. Materials Science and Technology, Pittsburgh, PA, October 28, 2009.

63. (Poster) "Modeling and experimental investigation of fracture behavior of pharmaceutical powder compacts." O. Keles, K. J. Bowman and R. E. García, Dane O. Kildsig,

Center for Pharmaceutical Processing Research, Industrial Advisory Board Meeting, Purdue University, November 16-18, 2009.

64. (Poster)"Microstructure Tailoring of Material Properties via Integrated Materials Processing and Computational Design." R. E. García and C. J. Martinez*. MCMA/DARPA Proposers' Day Workshop, Arlington, VA, December 17, 2009.

65. "Modeling and Optimization of Polymer-Based Bulk Heterojunction (BH) Solar cell," B. Ray*, P.R. Nair, and R. E. García, and M. Alam, International Electron Devices Meeting, Baltimore, MD, December, 2009.

66. "Modeling Ferroelectric Domain Polycrystalline Thin Films." R. E. García*. Electronic Materials and Applications, Orlando, FL, January 21, 2010.

67. "Modeling Rechargeable Batteries Through Finite Element Analysis." M. Smith, Q. Horn, and R. E. García*. Electronic Materials and Applications, Orlando, FL, January 21, 2010.

68. "Electromechanical Probing of Li-Activity on the Nanometer Scale in Cathode Materials." N. Balke*, S. Jesse, A. N. Morozovska, E. A. Eliseev, D.-W. Chung, R. E. García, Y. Kim, L. Adamczyk, N. J. Dudney and S. V. Kalinin. MRS, San Francisco, April 6, 2010.

69. (Poster)"Modeling and Characterization of $LiCoO_2$ through Scanning Probe Microscopy Method." D.-W. Chung*, S. Kalinin, N. Balke, R. E. García. Scanning Probe Microscopy for Energy Applications International Workshop, Oak Ridge National Laboratory, TN, September 2010.

70. "Mechanical Properties and Reliability of Pharmaceutical of Powder Processing Tablets: A Modeling Approach." O. Keles, R. E. García, K. J. Bowman. MS&T, Huston TX, October 2010.

71. "Modeling Polycrystalline Ferroelectric Population Dynamics." Z. Zhao,* C. Fancher, R. E. García, and K. J. Bowman. MS&T, Houston TX, October 2010.

72. "A Topological Study of Salient Structures in a High-Resolution Spheronization Simulation." N. Andrysco,* M. Koster, M. Thomes, R. E. García, and X. Tricoche. IEEE VisWeek, Salt Lake City UT, Oct 24-29, 2010.

73. "Modeling Domain Switching Population Dynamics in Polycrystalline Ferroelectrics." Z. Zhao*, C. Fancher, K. Bowman, R.E. García. EMA Orlando, FL, January 21, 2011.

74. "Ferroelectric Domain Switching Dynamics in Polycrystalline Thin Films." Z. Zhao, S. Leach, K. J. Bowman, and R. E. García*. Euromat 2011, Montpelier, France, September 12, 2011.

75. "Spatially Resolved Modeling of Rechargeable Battery Microstructures."

B. Vijayaraghavan*, R. E. García, and Y.-M. Chiang. Euromat 2011, Montpelier, France, September 12, 2011.

76. (Poster) "Gibbs: Symbolic Computation of Thermodynamic Properties and Phase Equilibria." T. Cool*, A. Bartol, M. Kasenga, K. Modi, and R. E. García*. Euromat 2011, Montpelier, France, September 13, 2011.

77. (Poster). "Local probing of ionic transport in energy storage materials." N. Balke, S. Jesse, S. Kalnaus, A. Morozovska, D.-W. Chung*, R. E. García, N. Dudney, C. Daniel, S. Kalinin. Gordon Research Conference, Batteries: Advanced Characterization, Theory and

Mechanisms of Processes in Rechargeable Batteries Across Length Scales. March, 2012, Four Points Sheraton, Ventura, California.

78. (Poster) "Level Set Modeling of Microstructure Evolution." Y. Wang*, D. R. Ely, D.-W. Chung, R.E. García. Gordon Research Conference, Batteries: Advanced Characterization, Theory and Mechanisms of Processes in Rechargeable Batteries Across Length Scales. March, 2012, Four Points Sheraton, Ventura, California.

79. (Poster) "Three Dimensional Simulation of Ultra High Energy Density Cathodes with Duplex Porosity." D. R. Ely*, Bharath Vijayaraghavan, Yet-Ming Chiang, R. Edwin García. Gordon Research Conference, Batteries: Advanced Characterization, Theory and Mechanisms of Processes in Rechargeable Batteries Across Length Scales. March, 2012, Four Points Sheraton, Ventura, California.

80. (Poster) "Virtual Electrochemical Strain Microscopy of Polycrystalline LiCoO2 Films," D.-W. Chung*, N. Balke, S. V. Kalinin, and R. E. García. Gordon Research Conference, Batteries: Advanced Characterization, Theory and Mechanisms of Processes in Recharge- able Batteries Across Length Scales. March, 2012, Four Points Sheraton, Ventura, California.

81. "Modeling of Porosity-Engineered Ultra High Energy Density Electrode Microstructures." B. Vijayaraghavan, H. Xie, D.-W. Chung, Y.-M. Chiang, R. García-García, and R. E. García*. 221st Meeting of the Electrochemical Society, Seattle, WA, May 10th, 2012.

82. "Spatially-Resolved Modeling of Three-Dimensionally Reconstructed Battery Electrode Microstructures." B. Vijayaraghavan, S. Harris, D.-W. Chung, R. García-García, and R. E. García. 221st Meeting of the Electrochemical Society, Seattle, WA, May 10th, 2012.

83. (Poster and 2nd Poster Meeting Highlight) "Mechanical and Electrical Reliability Maximization of Rechargeable Lithium-Ion Batteries through Microstructure Design." D.-W. Chung*, D. R. Ely, K. Feng, Y.-M. Chiang, B. Vijayaraghavan, and R. E. García. Gordon Research Conference, Solid Studies in Ceramics: New Insights and New Paradigms for Fracture and Deformation. Mount Holyoke College South Hadley, Massachusetts, August 2012.

84. (Poster and 1st Poster Meeting Highlight) "Statistical Failure Analysis of Crystallographically Isotropic Brittle Porous Materials." O. Keles*, R. E. García, and K. Bowman. Gordon Research Conference, Solid Studies in Ceramics: New Insights and New Paradigms for Fracture and Deformation. Mount Holyoke College South Hadley, Massachusetts, August 2012.

85. (Poster) "Microstructure Modeling of Ferroelectric Ceramics." Z. Zhao, S. E. Leach, Y. Saito, T. Tani, Y. Jing, X. Tricoche, G. Rohrer, J. Blendell, K. Bowman, and R. E. García*. Gordon Research Conference, Solid Studies in Ceramics: New Insights and New Paradigms for Fracture and Deformation. Mount Holyoke College South Hadley, Massachusetts, August 2012.

86. "Simulation and Design of (In,Ga)N-Based Light Emitting Diodes." Z. Liang, E. Stach, T. Sands, and R. E. García*. 222nd Meeting of the Electrochemical Society, Honolulu, HI, October 8th, 2012.

87. "Electrochemical and Mechanical Reliability of Three Dimensionally Reconstructed Electrode." R. E. García*. 222nd Meeting of the Electrochemical Society, Honolulu, HI,

October 11th, 2012.

88. (Poster) "Power Density and Reliability Correlations in LiCoO2 3D Laser-Structured Architectures." Daw Gen Lim*, Ding-Wen Chung, R Edwin García. Meeting Abstracts. 223rd Meeting of the Electrochemical Society, Toronto, Canada, May 12th-16th, 10:503, 2013.

89. "Tortuosity Anisotropy in Lithium Ion Battery Electrodes Studied by Synchrotron X-ray Tomography." Martin Ebner*, DW Chung, RE García, V Wood. Meeting Abstracts. 223rd Meeting of the Electrochemical Society. 10:409, 2013.

90. "Progress towards modeling microstructure evolution in polycrystalline films for solar cell applications." Y. Wang*, D.R. Ely, and R.E. García. Photovoltaic Specialists Conference (PVSC), 2013 IEEE 39th. 16-21 June 2013. 2056-2059.Tampa, FL.

91. (Poster) "Microstructure Modeling of Rechargeable Lithium-Ion Batteries." A. Jana*, and R. E. García. Gordon Research Conference, Batteries: Advances in Characterization, Analysis, Theory, and Modeling of Basic Processes. March 9-14, 2014. Four Points Sheraton/Holiday Inn Express, Ventura, CA.

92. (Poster) "The Effect of Microstructure on the Performance of Porous Li-Ion Electrodes." D.-W. Chung*, M. Ebner, D. R. Ely, O. R. Shearing, N. P. Brandon, S. J. Harris, V. Wood, and R. E. García. Gordon Research Conference, Ceramics, Solid State Studies in: Challenges Around Transport and Reactivity in Ceramics. July, 2014, Mount Holyoke College, Couth Hadley, MA.

93. (Poster) "Designing Safer Batteries by Suppressing Dendrite Growth." A. Jana*, D.R. Ely, and R. E. García. Gordon Research Conference, Ceramics, Solid State Studies in: Challenges Around Transport and Reactivity in Ceramics. July, 2014, Mount Holyoke College, Couth Hadley, MA.

94. (Poster) "Kinetics in High Energy Density Porous Electrode Battery Microstructures." R. Tu* and R. E. García. Gordon Research Conference, Ceramics, Solid State Studies in: Challenges Around Transport and Reactivity in Ceramics. July, 2014, Mount Holyoke College, Couth Hadley, MA.

95. (Poster) "An Analytical Description of Nanoparticle Dissolution Kinetics for Diffusion-Limited System." D.R. Ely*, M. Thomes, and R. E. García. American Association of Pharmaceutical Scientists. November 2-6, 2014, San Diego Convention Center, CA.

96. "Local Electromechanical Interaction Simulations Based on XRD-Determined Strains in Ferroelectrics." S.-Y. Song*, J. E. Blendell, and R. E. García. Electronic Materials and Applications 2015. January 21-23, Orlando, FL.

97. "Separator Design to Suppress Dendrite Growth in Lithium-Based Batteries" A. Jana*, D.R. Ely, and R. E. García. 227th ECS Meeting (May 24-28, 2015), Chicago, IL.

98. (poster) "Lithium Dendrite Suppression in Porous Rechargeable Li-Ion Batteries." A. Jana*, D.R. Ely, and R. E. García. 7th International Conference on Porous Media & Annual Meeting. Padova, Italy, May 18-20th, 2015.

99. "Dualfoil.py: A Li-ion Battery Simulation and Visualization Tool." L. D. Robinson*, and R. E. García. ORNL, Oak Ridge, TN, June 26th, 2015.

100. "Optimizing Electrode Microstructure Morphology." L. D. Robinson*, and R. E. García. 229th Meeting of the Electrochemical Society. San Diego, CA, May 29th-June 1st,

2016.

101. “Macroscopic Electrochemical Properties Starting from Spatially Resolved Electrochemical Data.” R. E. García. International Conference on Porous Media & Annual Meeting. Cincinnati, OH, May 8-12th, 2016.

102. “Phase Field Modeling of E-Field Assisted Sintering.” R. E. García. A Scientific Basis for Enhanced Manufacturability with Electrical Currents Basic Research Challenge Program Kick-off Meeting Evoke Logistics, 671 North Glebe Road, Arlington, 22203 VA, January 11th, 2017.

103. (Poster) “Effect of point defects on grain boundary phase transitions and coarsening in polycrystalline YSZ.” V. Karra* and R.E. García. Workshop on Electromagnetic Effects in Materials Synthesis. Carnegie Mellon University, Pittsburgh, PA, USA 5, 6 June 2017.

104. “The Effect of Charged Point Defects on the Grain Coarsening in Polycrystalline Ceramics.” V. Karra* and R.E. García. 21st International Conference on Solid State Ionics. Padua, Italy. June 18-23, 2017.

105. “Microstructural Limits and Extensions of Porous Electrode Theory.” A. Campos, I. Battiato, and R.E. García. 232nd Electrochemical Society Meeting. National Harbor, MD, Oct. 1-5, 2017.

106. “Meso and Microstructural Interactions in Porous Lithium-Ion Batteries.” A. Deva, and R.E. García. 232nd Electrochemical Society Meeting. National Harbor, MD, Oct. 1-5, 2017.

107. “Thermodynamics and Kinetics of Lithium Dendrite Growth.” A. Jana and R.E. García. 232nd Electrochemical Society Meeting. National Harbor, MD, Oct. 1-5, 2017.

108. “Grain Boundary Phase Transition Kinetics in Ionic Ceramics.” S. Karra*, W. Rheinheimer, M. Hoffmann, R.E. García MS&T, Pittsburgh PA, October 9th, 2017.

2.8 Invited Conference Presentations

1. “Microstructural Modeling and Design of Multifunctional Ceramics.” R. E. García*, W. C. Carter, Y.-M. Chiang, S. A. Langer, C. Bishop, P. Limthongkul, and M. Vaudin. 56th Pacific Coast Regional and Basic Science Division, Washington, Seattle, September 2004. (E.5.20)

2. “Microstructural Modeling and Design of Rechargeable Lithium-Ion Batteries.” R. E. García*, W. C. Carter, and Y.-M. Chiang. Meeting of the Electrochemical Society, Honolulu, Hawaii, October, 2004. (E.5.21)

3. “The Effect of Microstructure on the Domain Stability of Polycrystalline Ferroelectric PZT Films.” R. E. García*, J. E. Blendell, and B. Huey. PacRIM Meeting of the American Ceramics Society, Maui, Hawaii, September, 2005. (E.5.23)

4. “InGaN-Based Nanostructures for High-Performance Light Emitting Diodes” R. E. García*. American Ceramic Society, Daytona Beach, Florida, January, 2008. (E.5.39)

5. “The Effect of Microstructure on the Local and Macroscopic Switching of Polycrystalline Ferroelectric Films.” R. E. García*. The Minerals, Metals and Materials Society, New Orleans, March, 2008. (E.5.40)

2.8 Invited Conference Presentations

6 "The Effect of Crystallographic Texture on Ferroelectric Ceramics." R. E. García*. International Conference on Texture Materials, Pittsburgh, PA, June, 2008. (E.5.42)

7."The Effect of Microstructure on the Ferroelectric Switching of Polycrystalline Films." R. E. García*, E. Anton, J. Blendell, and K. Bowman Materials Science and Technology, October 2008. (E.5.44)

8."FiPy Round Table: Applications to Research and Education." R. E. García*. The Minerals, Metals and Materials Society, San Francisco, California, February 16, 2009. (E.5.46)

9."Status of Computational Materials Education in the US: Recent Results and Surveys." M. Asta,* K. Thornton, R. E. García. The Minerals, Metals and Materials Society, San Francisco, California, February 16, 2009. (E.5.48)

10. "Grain Boundaries-Ferroelectric Domains Interactions in Polycrystalline Ferroelectrics." S. Leach and R. E. García*. Materials Research Society, San Francisco, April 17, 2009.

11. "Grain Boundaries-Ferroelectric Domains Interactions in Polycrystalline Ceramics." Z. Zhao, C. Fancher, T. Cool, and R. E. García*. Vancouver, Canada, American Ceramic Society, PacRim Meeting 09, June 3, 2009. (E.5.58)

12. "Three-Dimensional Modeling of Piezoelectric Microstructures." S. Lee, T. Key, G. Rohrer, T. Tani, and R. E. García*. Materials Science and Technology, Sosman Symposium, Pittsburgh, PA, October 28, 2009. (E.5.61)

13. "Modeling Ferroelectric Domain Polycrystalline Thin Films." R. E. García*. Electronic Materials and Applications, Orlando, FL, January 21, 2010. (E.5.65)

14. "Modeling Rechargeable Lithium-Ion Batteries Through Finite Element Analysis." R. E. García*. Electronic Materials and Applications, Orlando, FL, January 21, 2011.

15. *"Microstructure Design of Lead-free Piezoelectric Ceramics."* R. E. García. MRS San Francisco, CA, April 28, 2011.

16. *"Microstructure Modeling of Rechargeable Lithium-Ion Batteries"* B. Vijayaraghavan, R. E. García*, and Y.-M. Chiang. ECS, Montreal, Canada, May, 5, 2011.

17. *"Microstructure Design of Lead-Free Piezoelectric Ceramics."* R. E. García*. ElectroCeramics XII, Stockholm, Sweden. June, 22, 2011.

18. *" Invisible: How Researchers Model Materials at the Nanoscale."* R. E. García*. Back to School, President's Council. West Lafayette, IN, September 30, 2011.

19. *"3D Simulation, Analysis, and Design of Rechargeable Li-Ion Battery Microstructures."* R. E. García*. Gordon Research Conference, Batteries: Advanced Characterization, Theory and Mechanisms of Processes in Rechargeable Batteries Across Length Scales. March, 2012, Four Points Sheraton, Ventura, California.

20. *"Validation, Data Management, and Visualization Challenges in the Simulation of 3D Battery Microstructures."* R. E. García*. NSF DMR Materials Genome Initiative Inaugural Workshop, February 22nd, 2013. Arlington, VA.

21. *"Electrochemical and Mechanical Reliability of Three Dimensionally Reconstructed Electrode Microstructures."* R. E. García*. TMS, 142nd Annual Meeting. March 4th, 2013. San Antonio, Texas.

22. *"Spatially Resolved Porous Electrode Theory for Rechargeable Lithium-Ion Battery Electrodes."* R. E. García*. TMS, 142nd Annual Meeting. March 4th, 2013. San Antonio,

Texas.

23. *"Modeling of Electrodes in Lithium-Ion Batteries."* R. E. García*. Computational Materials and Chemical Sciences Network (CMCSN) Workshop, April 15th, 2013, Purdue University, 2013.

24. *"Electrochemical and Mechanical Performance in Rechargeable Lithium-Ion Battery Electrodes."* R. E. García*. NEES-EFRC-online conference call, April 16th, 2013.

25. *"Electrochemical and Mechanical Reliability in Rechargeable Lithium-Ion Batteries."* R. E. García*. Canterbury, New Zealand, July 31st, 2013.

26. *"Spatially-Resolved Modeling of Three-Dimensionally Reconstructed Li-Ion Battery Electrode Microstructures."* R. E. García*. Institute for Pure & and Applied Mathematics. Workshop III: Batteries and Fuel Cells. San Diego, CA, November 6th, 2013.

27. *"Designing 3D Conical-Shaped Li-ion Micro-batteries."* D.G. Lim, D.-W. Chung, R. Kohler, J. Proell, C. Scherr, W. Pfleging, R. E. García*. TMS, 143rd Annual Meeting. Symposium: Nanostructured Materials for Rechargeable Batteries and Supercapacitors II. San Diego, California, February 17th, 2014.

28. "*Microstructural Aspects of Rechargeable Batteries: Performance and Degradation.*" R. E. García*. Gordon Research Conference, Batteries: Advances in Characterization, Analysis, Theory and Modeling of Basic Processes. March, 2014, Four Points Sheraton, Ventura, California.

29. "*Microstructural Aspects of Power Sources.*" R. E. García*. West Lafayette, IN. Purdue Fuel Cell Workshop, April 3rd, 2014.

30. "*Towards a General Microstructural Theory of Dendrite Nucleation and Growth in Rechargeable Lithium-Ion Batteries.*" R. E. García*. ETH, Zurich. April, 9th, 2014.

31. "*Phase Field Modeling and Electrochemical Systems: Applications to Rechargeable Li-Ion Battery Materials."* R. E. García*. Gordon Research Conference, Ceramics, Solid State Studies in: Challenges Around Transport and Reactivity in Ceramics. July 24th, 2014, Mount Holyoke College, Couth Hadley, MA.

32. "*Diseño Microestructural the Policristales Piezoeléctricos.*" R. E. García*. Seminario Sotero Prieto. Departamentos del Estado Sólido y Materia Condensada. IFUNAM. August 6th, 2014.

33. "*Charge Transport at the Mesoscale.*" R. E. García*. NEES-EFRC-online conference call, September 29th, 2014.

34. "*Concurrent Physical Vapor Deposition and Microstructure Evolution Simulation of Thin Films.*" Y. Wang, D. Ely, B.-J. Kim, E. Stach, and R. E. García*. MS&T, 2014, Pittsburgh, PA, October 15th, 2014.

35. "*The Effect of Microstructure in Rechargeable Li-Ion Battery Electrodes.*" R. E. García*. 7th International Conference on Porous Media & Annual Meeting. Padova, Italy, May 20th, 2015.

36. "*Phase Field Applications to Electrically Active Systems.*" R. E. García*. Interfaces, Stresses, and Stability: Learning from John W. Cahn. Islandwood, Bainbridge Island, WA, August 31st to September 4th, 2015.

37. "*Microstructural Modeling of Heterogeneous Nucleation and Growth of Lithium Elec-*

trodeposits." R. E. García*. 228th ECS Meeting, Phoenix, AZ, (October 11-15, 2015).

38. "Microstructural Degradation in Rechargeable Batteries." R. E. García. 229th Meeting of the Electrochemical Society. San Diego, CA, May 29th-June 2nd, 2016.

39. "*Microstructure Evolution and Properties of Polycrystalline Ceramics: A Phase Field Approach*." R.E. García. Ceramics, Solid State Studies in Gordon Research Conference: Creating Functionality of Advanced Ceramics by Innovative Materials Processing Mount Holyoke College South Hadley, MA, July 31 - August 5, 2016.

40. "Thermodynamic Stability and Transport Properties in Charged Grain Boundaries." V. Karra and R.E. García*. Workshop on Electromagnetic Effects in Materials Synthesis. Carnegie Mellon University, Pittsburgh, PA, USA 5, 6 June 2017.

41. "Equilibrium and Transport Properties in Charged Grain Boundaries." V. Karra and R.E. García*. 21st International Conference on Solid State Ionics. Padua, Italy. June 18-23, 2017.

42. "Grain Boundary Phase Transition Kinetics In Ionic Ceramics." V. Karra*, W. Rheinheimer, M. Hoffmann, R.E. García*. Symposium: Interfaces, Grain Boundaries and Surfaces from Atomistic and Macroscopic Approaches. Meeting: Materials Science & Technology, 2017. Pittsburgh, PA, October 8-12, 2017.

43. "Microstructural Evolution of Lithium Electrodeposits in Liquid Electrolytes." A. Jana*, and R.E. García. 2018 Conference on Electronic and Advanced Materials, Orlando, January 18, 2018.

44. "Properties and Microstructure Evolution of Materials with Electrically Charged Interfaces." R.E. García. Exploiting Defects and Interfaces in Paradigm-Shifting Processing and Extreme Environments, Gordon Research Conference: Solid State Studies in Ceramics. Mount Holyoke College, MA, USA, August 13th, 2018.

45. "Microstructurally-Induced Properties and Degradation in Lithium-Ion Batteries" R.E. García. XXVII International Materials Research Congress. Cancun, Mexico. August 22nd, 2018.

46. "Charged Grain Boundaries and the Microstructural Evolution of Ionic Ceramics." R.E. García. Materials Research Society, Fall Meeting, November 28th, 2018.

47. "Charged Interfaces and Microstructure Evolution of Ionic Ceramics." R.E. García. 2nd Topical Meeting SPP 1959, Bad Salzschlirf, Germany, December 4th, 2018.

2.9 Invited Colloquium and Seminar Series Presentations

1."Microstructural Design in Rechargeable Lithium-Ion Batteries." R. E. García*, C. M. Bishop, P. Limthongkul, W. C. Carter, S. A. Langer, and Y.-M. Chiang. George Mason University, September 2003.

2."Modeling Electrically Active Materials" Industrial Pharmacy Department, Purdue University. R. E. García*. May, 2006.

3."Microstructural Design", Proctor Academy, Andover, New Hampshire. August 2006.

4."Microstructure Engineering of Fusing Materials and Devices." Littelfuse. Chicago, Illinois. R. E. García*. August, 2006.

5.“Microstructure Design of Electrically Active Materials.” Department of Materials Science and Engineering, Carnegie Mellon University. R. E. García*. May, 2007.

6.“Microstructural Design of Electrically Active Materials and Devices Through Computational Modeling: The OOF Project.” ECE Department, Purdue University. R. E. García*. June, 2007.

7.“Modeling the Effect of Microstructure of Rechargeable Lithium-Ion Batteries.” R. E. García*. Medtronic, Minneapolis, Minnesota January, 2008.

8.“The Effect of Microstructure on the Ferroelectric Switching of Polycrystalline Ferroelectrics.” R. E. García*.Darmstadt Technical University, Darmstadt, Germany, May, 2008.

9.“Modeling the Effect of Microstructure of Rechargeable Lithium-Ion Batteries.” R. E. García*. Darmstadt Technical University, Darmstadt, Germany, May, 2008.

10.“Next Generation Energy Sources through Microstructure Design.” R. E. García*. IUPUI, IN, September, 2008.

11.“Microstructure Design of Portable Power Sources through Object Oriented Finite Elements.” R. E. García*, M. Smith, and K. Yamamoto. Lovell Symposium, Purdue University, October 2008.

12.“Supporting Connections Between Research and Learning - Materials Digital Library (MatDL).” L. Bartolo, J. Warren, R. E. García*. (webinar - seminar on line) February 5th, 2009.

13.“Next Generation Rechargeable Batteries through Microstructure Design.” R. E. García*. Battery Workshop: What can Indiana do to be a Leader in Battery Technology.” Purdue University, February 26, 2009.

14.“Modeling Cool Stuff.” R. E. García* and A. Strachan*. Purdue MSE, Friday Seminar. March 13, 2009.

15.“Microstructure Modeling and Design of Power Sources.” R. E. García*, M. Smith, and K. Yamamoto. The McLaren Symposium (Ed Fuller). Rutgers University, March 27, 2009.

16.“Grain Boundaries-Ferroelectric Domains Interactions in Polycrystalline Ceramics.” Z. Zhao, C. Fancher, T. Cool, and R. E. García*. Darmstadt, Germany, May 20, 2009.

17.“Modeling and Design of Materials and Devices.” R. E. García*. University of Karlsruhe, Karlsruhe, Germany, May 26, 2009.

18.“Microstructure Modeling and Design of Power Sources through Object Oriented Finite Elements.” R. E. García*. Toyota US Research and Development, Detroit, MI, August 28, 2009.

19.“Microstructure Modeling and Design of Rechargeable Batteries.” R. E. García*. Central Michigan University, MI, September 25, 2009.

20.“Model Development for Understanding Mechanical Properties of Powder Compacts II: Design of Milling for Roller Compacted Ribbons.” K. J. Bowman and R. E. García*, Dane O. Kildsig , Center for Pharmaceutical Processing Research, Industrial Advisory Board Meeting, Purdue University, November 16-18, 2009.

21. “Microstructure Modeling and Design of Rechargeable Batteries.” R. E. García*. GE Global Research Albany, NY, December 7, 2009.

2.9 Invited Colloquium and Seminar Series Presentations

22."Continuum Modeling of GaN Nanostructures for Electronic Devices Applications." R. E. García*. U.S. Army Research Laboratory, MD, March 17, 2010.

23."Three-Dimensional Modeling of Piezoelectric Microstructures." Z. Liang, S. Lee, T. Key, S. Wang, G. Rohrer, X. Tricoche, and R. E. García*. Toyota TEMA, Nagoya, Japan, June 7, 2010.

24."Microstructure Modeling and Design of Rechargeable Lithium-Ion Batteries.*"* W.-D. Chung, B. Vijayaraghavan, Z. Liang, M. Smith, and R. E. García*. Toyota TEMA, Nagoya, Japan, June 10, 2010.

25."Modeling of Ferroelectric Polycrystals," R. E. García*. Technische Universität Darmstadt, Darmstadt, Germany, July 21, 2010.

26."Modeling and Design of Material Microstructures," Purdue Center for Predicted Materials Modeling and Simulation workshop, August 10-11, 2010.

27. "Microstructure Design of Lead-Free Piezoelectric Ceramics," R. E. García*. University of Michigan, Ann Arbor, MI, September 10, 2010.

28. "III-Nitride Nanopyramids for LED Applications." R. E. García*. Workshop on NIST, Gaithersburg, MD, September 30, 2010.

29. *"Simulation and Design of (In,Ga)N-Based Light Emitting Diodes."* Z. Liang, R. E. García, R. Colby, E.A. Stach, I. Wildeson, D. Ewoldt, D. Zakharov, J. L. Schroeder, and T. D. Sands RPI, Albany, NY, October 5, 2011.

30. "*CS Challenges and Opportunities in the Design of Rechargeable Batteries.*" R. E. García. Interdisciplinary Graduate Programs. CSE/CLS Seminar. Purdue University, West Lafayette, IN, September 17th, 2014.

31. "Degradation in Rechargeable Li-Ion Batteries." R. E. García. LAAST Seminar. Purdue University, West Lafayette, IN, February 12th, 2015.

32. "Modeling and Simulation of Lithium-Ion Batteries." R. E. García. CCAM Seminar. Purdue University, West Lafayette, IN, March 6th, 2015.

33. "Microstructure Design of Rechargeable Battery Electrodes." R. E. García. Crane Naval Surface Warfare Division. Bloomington, IN. May 14th, 2015.

34. "Microstructural Performance in Rechargeable Batteries." R. E. García. IEK Colloquium. Jülich, Germany, June 12th, 2015.

35. "Progress Towards a Microstructurally Resolved Porous Electrode Theory." R. E. García. ORNL, Oak Ridge, TN, June 26th, 2015.

36. "Microstructural Modeling of Lithium-Ion Rechargeable Batteries." R. E. García. 7th STFC Global Challenge Network in Batteries and Electrochemical Energy Devices. Annual Meeting. Cosener's House Abingdon, England. 30th June/1st July, 2015.

37. "*The Effect of Microstructure in Rechargeable Lithium-Ion Batteries.*" R. E. García. UIC/JECSR Workshop on Advanced Batteries Research University of Illinois Chicago October 15-16, 2015.

38. "Status of Rechargeable Lithium-Battery Technology." R. E. García. Purdue University Retiree Association. March 7th, 2016.

39. "The Effect of Microstructure on the Energy Density of Rechargeable Li-Ion Batteries." R. E. García. San Diego State University. June 3rd, 2016.

2.9 Invited Colloquium and Seminar Series Presentations

40. "The Effect of Microstructure on the Multifunctional Properties of Ceramics." R. E. García. Sandia National Labs. Albuquerque, NM, August 30th, 2016.

41. "Properties and Microstructure Evolution of Granular Materials of Energy-Related Applications." R. E. García. Kaiserslautern TU, Kaiserslautern, Germany, October 17th, 2016.

42. "The Effect of Microstructure on the Properties of Polycrystalline and Porous Materials." R. E. García. Dortmund TU, Dortmund, Germany, October 19th, 2016.

43. "Properties, Transport, and Microstructural Evolution in Granular Materials for Energy Applications." R. E. García. Stanford University, Stanford, CA, January 27th, 2017.

44. "Propiedades, Transporte de Carga, y Evolución Microestructural en Materiales Granulares para Aplicaciones Energéticas." (Properties, Charge Transport, and Microstructural Evolution for Energy Applications) R.E. García. Institute of Materials, UNAM, May 29th, 2017.

45. "Meso and Microstructural Interactions in Porous Lithium-Ion Batteries." R.E. García. Stanford University, Stanford, CA, January 23rd, 2018.

46. "Lithium Dendrite Growth in Rechargeable Batteries." R.E. García. University of Canterbury, Christchurch, New Zealand, May 17th, 2018.

47."Charged Grain Boundaries in Ionic Ceramics." R.E. García. University of Canterbury, Christchurch, New Zealand, June 11th, 2018.

3 Technology Transfer

3.1 Summary

3.1.1 Introduction

Prof. García has contributed to the development of several scientific software applications to simulate properties, structure, performance or microstructural evolution of materials. These four major areas summarize the wide interdisciplinary nature of Materials Science, which aims to understand and engineer the chemical and physical characteristics and properties of new substances and devices by optimizing their final form. The associated software packages were published in nanoHUB.org, matforge.org, nist.gov, and matdl.org.

3.1.2 The Object Oriented Finite Element Analysis

OOF provides a unique framework to learn, discover, and engineer the performance of materials and devices of complex geometries. This easy-to-use Finite Element framework allows to create complex numerical representations of materials and devices directly from images, simultaneously identifying boundaries and edges and bringing the finite element mesh into correspondence with the topological features of the mesh. With a unique portfolio of image-based, adaptive meshing techniques, OOF and OOF2 are capable of parsing experimental data relating to materials with complex geometries into representations that are amenable for the description of elastic, thermal, and piezoelectric systems.

3.1.3 The Virtual Kinetics of Materials Laboratory

VKML, and VKML-Live are a cloud-enabled infrastructure that empowers current ad future generations of engineers to rapidly prototype numerical models to design new material models, devices, and processing operations. While its most basic infrastructure allows you to simulate grain growth and coarsening, dendrite formation, ferroelectric switching, and spinodal decomposition, the available advanced tools allows the user to create phase field models to numerically represent any microstructural evolution and processing of advanced materials and devices. Such tools have been introduced in graduate and undergraduate level numerical modeling courses (MSE 597I and MSE 597G) and have led to the development and publication of tutorials and workshop lectures at important forums such as MRS, TMS and MS&T.

3.1.4 Gibbs and Gibbs-Live

Gibbs is a python-based symbolic infrastructure that allows to rapidly prototype advanced theories and models to assess the thermodynamic stability, equilibrium properties, and multiphysical response of currently existing and emerging materials. The importance of this very recent contribution is key for the Materials Science community for the increasing demand to integrate effective microstructure design methods with multicomponent alloys prediction, to improve both the design of alloys and the design of processes for producing materials with unique properties.

3.2 Patents Awarded

- G. R. Maskaly, Y.-M. Chiang, W. C. Carter, and R. E. García *"Ionic Colloidal Crystals."* US Patent 7,446,130 B2. Nov. 4, 2008.
- L. Robinson and R. E. García "Rechargeable Battery Electrodes having Optimized Particle Morphology." US Patent 15610619, March, 22, 2018.

3.3 Patents and Copyrights Submitted

1. B. W. Boudouris, E. Marinero, and d R. E. García. "Terpolymer-Derived Membranes as Battery Separators." Provisional US Patent 66579, February, 2014.
2. R. Ely, A. Jana, and R. E. García. "Dendrite Growth Simulation Simulation System and Method." Provisional US Patent 66760-01 July, 2014.
3. Y. Wang, D.R. Ely, and R. E. García. "Method for Physical Vapor Deposition of Thin Film Microstructures." Provisional US Patent 66759-01 July, 2014.
4. D. Ely, A. Jana, and R. E. García. "Dendrite Growth Simulation Framework for the Design of Battery Materials." 1-3263948281 April, 2016.
5. R. E. García. "Batts3D: Three-Dimensional Simulation of Battery Materials." Provisional US Patent **2016-GARC-**67575 August, 2016.
6. L. Robinson and R. E. García "Rechargeable Battery Electrodes." Provisional US Patent 66758-01 August, 2014.
7. "cMorph: Scientific Software for the Large Chemomechanical Deformation and Microstructure Evolution of Battery Materials." R. E. García , A. Jana, S. Woo, V. Karra. Copyright # 1-3839397101. July, 2016.

4 Teaching

4.1 Summary

The effort has focused on the development of undergraduate and graduate human resources with a deep understanding of the properties and microstructure evolution of materials in order to face the engineering challenges of the future. Elements of numerical modeling have been introduced in the undergraduate and graduate curriculum to empower students with intellectual tools to engineer the properties and performance of materials and devices. Integration of advanced scientific concepts and mathematical tools to the students' natural intuition in the context of open-ended problem solving skills has been developed in four strategic areas: **a)** Computational Materials, **b)** Thermodynamics of Materials, and **c)** Kinetics of Materials **d)** Rechargeable Battery Materials.

4.2 New Courses Introduced at Purdue

Title: MSE597G *Modeling and Simulation of Materials*
Date introduced and taught: (Fall 2006, Fall 2008, Fall 2010)
Enrollment history: 17 (Fall 2006), 14 (Fall 2008), 13 (Fall 2010)
Percentage of responsibility: 50%
Preparation of instructional materials: co-authored, 17 Lectures, 4 Homework assignments and nanoHUB-based teaching materials (https://nanohub.org/groups/mse597g/wiki)

Title: MSE 597I *Introduction to Computational Materials*
Date introduced and taught: (Fall 2007, Fall 2009, Fall 2011, Spring 2014)
Enrollment history: 13 (Fall 2007), 17 (Fall 2009), 17 (Fall 2011), 14 (Fall 2014)
Percentage of responsibility: 100%
Preparation of instructional materials: 38 Lectures, 4 Homework assignments, teaching software:

- https://nanohub.org/tools/gibbs,
- https://nanohub.org/tools/oof2,
- https://nanohub.org/tools/vkmllive,
- https://nanohub.org/tools/vkmlggs/,
- https://nanohub.org/tools/vkmlpsgg/,
- https://nanohub.org/tools/vkmlsd/,
- https://nanohub.org/tools/vkmlsd3d/ ,

4.2 New Courses Introduced at Purdue

nanoHUB-based teaching materials:

- https://nanohub.org/groups/mse597i ,
- https://nanohub.org/groups/mse597introductiontocomputationalmaterials2011,
- https://nanohub.org/groups/computationalmaterials2014.

Title: MSE 597N *Physical Properties of Crystals*
Date introduced and taught: (Fall 2008, Fall 2010)
Enrollment history: 7 (Fall 2008), 37 (Fall 2010)
Percentage of responsibility: 50%
Preparation of instructional materials: co-authored, 23 Lectures, 4 Homework assignments.

Title: MSE 597GM *Introduction to the Materials Science of Rechargeable Batteries*
Date introduced and taught: (Spring 2010, Spring 2011, Fall 2012, Fall 2013, Fall 2015, Fall 2017)
Enrollment history: 16 (Spring 2010), 15 (Spring 2011), 22 (Spring 2012), 17 (Fall 2013), 45 (Fall 2015), 13 (Fall 2017)
Percentage of responsibility: 50% on Spring 2010; 100% thereafter.
Preparation of instructional materials: 24 Lectures, 4 Lecture assignments,
term project, nanoHUB-based teaching materials:

- https://nanohub.org/groups/mse597rb,
- https://nanohub.org/groups/mse597batterymodeling,
- https://nanohub.org/groups/mse597rb_2013,
- https://nanohub.org/groups/mserechargeablebatteries,
- https://nanohub.org/groups/mserechargeablebatteries2015,
- https://nanohub.org/groups/mserechargeablebatteries2017.

Title: MSE 597K *Kinetics of Materials*
Date introduced and taught: (Fall 2014)
Enrollment history: 14 (Fall 2014), 12 (Spring 2017)

4.3 Courses Taught

Title: MSE230 *Structure and Properties of Materials* Lead: D. Johnson. Teaching Assistants: R. E. García, C. A. Handwerker

Semester and year: Fall 2005
Enrollment: 77
Percentage of responsibility: 25%

Title: MSE 430 *Materials Process and Design I.*
Semester and year: Fall 2005
Enrolment: 5
Percentage of responsibility: 100%

Title: MSE 440 *Materials Process and Design II*
Semester and year: Spring 2006
Enrollment: 5
Percentage of responsibility: 100%

Title: MSE350 (currently MSE 260) *Thermodynamics of Materials*
Enrollment history:
Spring 2006; 30 students; 50% responsibility
Spring 2007; 32 students; 100% responsibility
Spring 2008; 57 students; 50% responsibility

Title: ENGR103 *Next Generation Materials for Energy and Electronics*
Semester and year: Fall 2007 Lead: C. A. Handwerker. Assisted: J. E. Blendell, K. Trumble, R. E.
García, A. Strachan.
Enrollment: 28
Percentage of responsibility: 25%

Title: MSE 260 (previously MSE350) *Thermodynamics of Materials*
Enrollment history:
Spring 2009; 60 students; 100% responsibility
Spring 2010; 47 students; 100% responsibility
Spring 2012; 52 students; 100% responsibility
Spring 2013; 69 students; 100% responsibility
Spring 2015; 63 students; 100% responsibility

Spring 2016, 47 students; 100% responsibility
Fall 2016, 15 students; 100% responsibility

Title: MSE190 *Introduction to Materials Engineering*
Enrollment history:
Spring 2008; 19 Students; 100% responsibility
Fall 2009; 16 students; 100% responsibility
Fall 2011; 33 students; 100% responsibility

4.4 Major PhD and MS Advisor

Advised graduate students					
Name	Degree	Graduation Date	Name of Co-Chair	Title	Related Publications (section 2.2)
Mara J. Howell	MS	08/07	Tim Sands	Engineering the Thermoelectric Behavior in Nanodots, Nanowires, and polycrystalline Materials	
Kei E. Yamamoto	MS	05/08	None	Microstructural Design of Solid Oxide Fuel Cells	
David Robert Ely (IPPH)	PhD	05/10	Teresa Carvajal	Characterization of Dry Powder Segregation and Flowability: Experimental and Numerical Studies	33, 35, 42, 44, 47, 48, 49
Zhiwen Liang	PhD	12/10	None	Simulation and Design of (In,Ga)N-Based Light Emitting Diodes	20, 22, 25, 27, 28, 34

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Table 1: continued...

Name	Degree	Graduation Date	Name of Co-Chair	Title	Related Publications (section 2.2)
Sarah Leach	PhD	12/14	None	Edge and Finite Size Effects in Polycrystalline Ferroelectrics	17, 21, 26, 45
Zizhao Zhao	PhD	05/12	None	Modeling Domain Switching Population Dynamics in Polycrystalline Ferroelectrics	32, 52
Ozgur Keles	PhD	05/14	Keith Bowman	Model Development to Understand Mechanical Properties of Powder Compacts	36, 37, 43, 46, 46, 53
Bharath Vijayaraghavan	MS	01/12	None	Mechanical and Electrical Reliability Maximization of Rechargeable Lithium-Ion Battery Microstructures	33
Ding-Wen (Tony) Chung	MS	07/13	None	The Effect of Microstructure on the Performance of Li-Ion Porous Electrodes	24, 30, 38, 39, 41

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Table 1: continued...

Name	Degree	Graduation Date	Name of Co-Chair	Title	Related Publications (section 2.2)
Yunbo Wang	MS	12/13	None	Phase Field Modeling of the Physical Vapor Deposition of Thin Film Microstructures	44
Aniruddha Jana	PhD	08/19	None	Modeling the Microstructure Evolution of Electrochemically Active Systems	47, 49, 57, 59 65
Vikrant Suryanarayana Karra	PhD	12/19	None	Phase Field Modeling of Electric Field-Assisted Sintering	58, 60, 61, 62, 64
Abhas Deva	PhD	12/20	None	Spatially Resolved Microstructural Properties of Batteries	
Juan Alfonso Campos	PhD	05/21	None	Averaged Microstructural Properties of Batteries	
Lucas Robinson	PhD	12/21	None	Microstructural Properties of Solid State Batteries	
Jarrod Lund	PhD	12/21	None	Thermodynamics and Kinetics of Electrochemical Systems	

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Table 1: continued...

Name	Degree	Graduation Date	Name of Co-Chair	Title	Related Publications (section 2.2)
Surya Mitra	PhD	12/22	None	Electrochemistry and chemomechanics of Materials	

4.5 Visiting Scholars and Postdoctoral Researchers

Advised graduate students					
Name	Last Degree Date	Prior Affiliation	Position/Dates	Project Title	Related Publications
Sukbin Lee	PhD/2009	Carnegie Mellon University, USA	Postdoc 06/01/09 - 05/31/10	Analyses of Textured Piezoelectric Ceramics	34
Martin Koester	BD/2009	Institut fur Pharmazeutische Technologie und Biopharmazie Heinrich-Heine-Universitat, University of Dusseldorf, GE	Visiting Scholar 12/01/2009-06/30/2010	DEM Modeling of Dry Particle Mixtures for Pharmaceutical Applications	48
Eva Maria Anton	BD/2009	Darmstadt Technical University, GE	Visiting Scholar 02/2007-05/2008	Domain Switching Mechanisms in Polycrystalline Ferroelectrics with Asymmetric Hysteretic Behavior	18

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Table 2: continued...

Name	Last Degree Date	Prior Affiliation	Position/Dates	Project Title	Related Publications
David R. Ely	PhD/2010	Purdue University, USA	Postdoc 04/01/2011-05/01/2013	Integrated Computational Materials Modeling of Magnesium Anode Electrodes	33, 35, 42, 44, 47, 48, 49
Catherine M. Bishop	PhD/2003	University of Canterbury, NZ	Visiting Faculty	Cyclic Degradation in Textured Ferroelectric Ceramics	2, 3, 4, 63
Sang Inn Woo	PhD/2015	Purdue University, USA	Postdoc 09/15/2015-	Modeling and Design of Composite Separators for Li-Ion Batteries	
Alfredo San Juan	PhD/2017	National University of Mexico, Mexico	Postdoc 10/29/2018-	Modeling of charged droplet dynamics	

4.6 M. S. Advisory Committee

1. Kevin Grossklaus (MSE) Graduation date: 07/2007.
2. Brian Piccione (MSE) Graduation date: 07/2007.
3. Guojing Huo (MS-NUCL). Graduation date: 05/2010.
4. Patrik Rajanbhai Halanai. Graduation date: 05/2011.
5. Oluwatosin Ogunwuyi (CIT). Graduation date: 08/2013.
6. Sean Evan Wisniewski Sullivan. Graduation date: 05/2013.
7. Guijing Huo (NUCL). Graduation date: 05/2016.

4.7 Ph. D. Advisory Committee

1. Wonyoung Chang (MSE). Graduation date: 08/2007.

2. Mahidar Rayasam (ME). Graduation date: 05/2007.
3. Kaushik Srinivasa (ME). Graduation date: 05/2009.
4. Jon Paul Tucker (MSE) Graduation date: 05/2009.
5. Woo-Suhl Cho (MSE-CE) Expected graduation date: 08/2010.
6. Hung-Yun Lin (MSE). Expected graduation date: 05/2013.
7. Lea Kristelle Marlor (MSE). Expected graduation date: 05/2011.
8. Meredith Elisa Dubelman (MSE). Expected graduation date: 05/2012.
9. Nathan Lawrence Anderson (MSE). Expected graduation date: 05/2012.
10. Francoise B. Angoua (MSE). Expected Graduation Date: 12/2010.
11. Patrick Robert Cantwell (MSE). Expected graduation date: 05/2011.
12. Robert Jason Colby (MSE). Graduation date: 05/2011.
13. Yuanyuan Jing (MSE) Expected graduation date: 12/2010.
14. John P. Koppes (MSE) Expected graduation date: 12/2011.
15. Oluwole Morgan (ME) Expected graduation date: 12/2011.
16. Sonal Shivaji Padalkar (MSE) Graduation date: 05/2010.
17. Subramanya Gautam Sadasiva (ME). Expected graduation date: 05/2012.
18. Muhammad Usman (EE). Expected graduation date: 08/2010.
19. Abhishek Ramish Tambat (ME). Expected graduation date: 08/2011.
20. Jonathon Paul Tucker (MSE). Expected graduation date: 08/2011.
21. Isaac Harshmamn Wildeson (ECE). Expected graduation date: 12/2010.
22. Al-Montaser Ahmad Al-Ajlony (NUCL). Expected graduation date: 08/2013.
23. Ghadeer Hamseh Al-Malkawi (NUCL). Expected graduation date: 05/2014.
24. Lei Cao (ME). Expected graduation date: 05/2015.
25. Matthias Claudius Ehmke (MSE) Expected graduation date: 05/2013.
26. Keng-Hua Lin (MSE) Expected graduation date: 08/2014.
27. Abhishek Ramesh Tambat (ME) Expected graduation date: 08/2014.

28. Mitchell Anthony Wood (MSE) Expected graduation date: 05/2015.
29. Xue Yang (MSE) Expected graduation date: 12/2013.
30. Wei-Hsun Chen (MSE). Expected graduation date: 05/2013.
31. Keng-Hua Lin (MSE). Expected graduation date: 08/2014.
32. Xiao Ma (MSE) Expected graduation date: 05/2014.
33. Hee-Joon Chun (ChemEng) graduation date: 05/2017.
34. Rong Xu (ME) graduation date: 05/2018.
35. Karim Elsayed Abdel A Ahmed (NucE) graduation date: 05/2015.
36. Mauricio David Guzman (MSE) graduation date: 05/2015.
37. Cheol Woong Lim (ME) graduation date: 05/2015.
38. Samuel T. Reeve (MSE) graduation date: 05/2017.
39. Camilo Vieira Mejia (Technology) graduation date: 05/2015.
40. Hee-Joon Chun (ChemE) graduation date: 05/2017
41. Daw Gen Lim (MSE) graduation date: 08/2018
42. Waterloo Tsutsui (AAE) graduation date: 05/2017
43. Rajath Kantharaj (ME) graduation date:05/2021
44. Tridib Kumar Saha (ME) graduation date: 12/2018
45. Vaidehi Hoshing (ME) graduation date: 12/2018
46. Hong Sun (-) graduation date: 12/2019
47. Rong Xu (-) graduation date: 05/2018
48. Keisuke Yazawa (MSE) graduation date: 05/2020
49. Han Yazawa (MSE) graduation date: 12/2018
50. Zhimin Qi (MSE) graduation date: 12/2019
51. Sritapaswi Nori (MSE) graduation date: 05/2020
52. Megan Rachel Kephart (MSE) graduation date: 05/2019
53. Jaehun Cho (AAE) graduation date: 05/2020

54. Megan Rachel Kephart (MSE) graduation date: 05/2019
55. Rajath Kantharaj (ME) graduation date: 05/2021
56. Bing Li (AA) graduation date:08/2020
57. Sritapaswi Nori (MSE) graduation date: 05/2020
58. Zhimin Qi (MSE) graduation date: 05/2020
59. Tridib Kumar Saha (EE) graduation date: 12/2018
60. Derek Karl Wittenburg Schwanz (MSE) graduation date: 05/2018
61. Hong Su (ME) graduation date:12/2019
62. Han Wang (MSE) graduation date 12/2018
63. Robert E. Warburton (ChemE) graduation date:08/2019
64. Keisuze Yasawa (MSE) graduation date: 05/2020
65. Oscar Torres Mattheus (ME, University of Canterbury, New Zealand) graduation date: 08/2019
66. César Augusto Martínez SÁnchez (PHYS, National University of Mexico) graduation date: 08/2020

4.8 Undergraduate Projects

Directed undergraduate projects contribute to seven publications in peer-reviewed journals and four nanoHUB, software publications.

1. Matthew Kasenga. MSE 499. *"Phase Diagram Modeling of Nanomaterials."* Fall 2006, Fall 2007. Developed proof-of-concept algorithms to predict binary phase diagrams. Developed fundamental proof-of-concept algorithms to accelerate the calculation of commercially relevant phase diagrams (related publications: E1-22, E4-4).

2. Heather Murdoch. MSE 499. *"Texture Engineering of Ferroelectric Materials."* Spring 2007. Analyzed the effect of texture in a thin-film, PZT-based ferroelectric thin-film. Proposed optimal texture parameters to maximize Random Access Memory applications (related publications: E1-15).

3. Madeleine Smith. MSE 499. *"Modeling Real Microstructures in Lithium Cobalt Oxide Based Rechargeable Batteries."* Fall 2007, Spring 2008. Analyzed the effect of microstructure, randomness, and particle size in a real rechargeable battery (related publications: E1-19).

4. Jackie Bernhard. MSE 499. *"Texture and Crystallographic Anisotropy Effects in Lithium Iron Phosphate-Based Cathode Electrodes."* Fall 2007, Spring 2008. Explored the effect of crystallographic texture for LiFePO4 composite battery architectures.

5. Katherine Frank. MSE 499. *"Triple Phase Boundary Modeling of LSM-Based Solid Oxide Fuel Cells."* Fall 2007, Spring 2008. Explored several analytical models to simulate a Solid Oxide Fuel Cell.

6. Michael Waters. MSE 499. *"Phase Field Modeling of Dendrites in Rechargeable Lithium-Ion Battery Electrodes."* Fall 2007, Spring 2008. Summer 2008 (SURF). Developed the Virtual Kinetics of Materials Laboratory, version 1, by using RAPPTURE. Four kinetic models were developed: Grain Growth, Spinodal Decomposition, Spinodal Decomposition 3D. and Dendrite Growth (related publications: E4-2).

7. Prakit Mohal. SURF. *"Modeling Of Thermal Stresses Effects in Solid Oxide Fuel Cells."* Summer 2007. Analyzed the effect of microstructure in a real Solid Oxide Fuel Cell. The developed model explicitly includes the effects of porosity and randomness for a YSZ-based cathode.

8. Thomas Cool. MSE 499. *"Tailoring of Ferroelectric Domains."* Fall 2008, Spring 2009. Developed Matplotlib-based visualization tools to analyze the effect of stress in polycrystalline ferroelectrics.

9. Christopher Fancher. MSE 499. *"Tailoring of Ferroelectric Domains."* Fall 2008, Spring 2009. Analyzed the effect of grain boundaries during ferroelectric switching in a polycrystalline PZT sample.

10. Alexander Bartol. *"Python-Based Rapid GUI prototyping for Thermodynamics and Kinetics of Materials Research Applications and Educational Demos."* Spring 2009, Summer 2009, Fall 2009, Spring 2010. Developed a TKInter-based GUI library to rapidly prototype materials science applications for education and research programs (related publications: E4-2, E4-3, E4-4).

11. Kunal Modi. SURF. *"Gibbs: Symbolic Computation of Thermodynamic Properties and Phase Equilibria."* Summer 2009 Developed an accelerated C-based algorithm to predict a binary phase diagram (related publications*:* E4-4).

12. Thomas Cool. *"Gibbs: Symbolic Computation of Thermodynamic Properties and Phase Equilibria."* Fall 2009. Created symbolic infrastructure to assemble thermodynamic models to predict generalized phase diagrams where stress, and size effects for classic materials, nanomaterials, and rechargeable battery materials *(related publications:* E1-22, E4-4, E4-5).

13. Ambrosius Limiadi. MSE 499. *"Modeling of Transport Properties of LiFePO4-Based Electrode Materials."* Fall 2009, Spring 2010. Developed a numerical framework to predict chemical diffusivities of materials by starting from the natural atomic vibrational frequencies of the individual atoms.

14. Ding-Weng (Tony) Chung. MSE 499. *"Nanometer-Scale Electrochemical Intercalation and Diffusion Mapping of Li-Ion Battery Materials."* Fall 2009, Spring 2010, Summer 2010. Explained the effect of surfaces and interfaces, bulk diffusion, and crystallographic anisotropy on the intercalation dynamics of LiCoO2 thin-film layers (related publications: E1-23).

15. Michael Johnston. MSE 499. *"Intercalation Dynamics and Phase Separation in $LiFePO_4$ Particles for Battery Applications."* Fall 2009, Spring 2010. Explored an alternate

model to simulate the intercalation dynamics of one of the most important emerging battery chemistries.

16. Rajiv Bharat Pithadia. MSE 499. *"Finite Element Modeling of 3D Battery Architectures."* Spring 2010. Explored through numerical modeling optimal battery architectures to maximize battery performance. Analyzes suggest an increase of a factor of two for the proposed architectures.

17. Peter McCallum. MSE 499. *"OOF Modeling of Material Microstructures."* Spring 2010. Studied the effect of microstructure in composite magnetoelectric materials. Started from experimental PFM images and reconstructed the polarization distribution as a function of magnetolectric stimulus.

18. Nik Maxwell. SURF. "*Web-Based Visualization of Material Properties.*" Summer 2010. Developed Open Source Web-Based Framework to automatically generate a website that presents scientific results, by starting from a set of unformatted data.

19. Di Hu. SURF "*Modeling of Piezoelectric Microstructures.*" Summer 2010. Studied the effect of texture and crystallographic anisotropy on the macroscopic electromechanical behavior.

20. Garret Nave. MSE 499 "Mathematica-Based Modeling of Rechargeable Lithium-Ion Batteries." Developing link between existing numerical battery models and analytical models being developed by Tian Qiu

21. Tian Qiu. MSE 499. "Analytical Modeling of Rechargeable Lithium-Ion Batteries." Spring 2011. Currently exploring analytical means to describe the battery response of UHED batteries.

22. Gamini Mendis MSE 499 "Modeling Texture Effects in Lead-Free Piezoelectric Microstructures." Fall 2010, Spring 2011. Developing a two-dimensional Finite Element formulation to simulate the effect of microstructure in BT, BNT, and BNKT-based ceramics in order to compare how valid they are with respect to full-fledged three-dimensional models.

23. Garret S. Nave. MSE 499 "Modeling of Ferroelectric Memories andor Actuators" Fall 2010.

24. Haochen Xie. MSE 499 "Modeling the two-phase intercalation behavior in battery particles of arbitrary shape." Fall 2011, Spring 2012.

25. Keng Feng . MSE 499 "Ultra High Energy Density Batteries." Spring 2012.

26. Benjamin Hester. MSE 499 "OOF Literature Search." Spring 2012.

27. Daw Gen Lim. MSE 499 "Nanodot Based Batteries." Spring 2012, SURF-Summer 2012, Fall 2012, Spring 2013.

28. Chloe Heinen. MSE 499 "Tortuosity in Batteries." Fall 2012, Spring 2013.

29. Matthew Lancaster. MSE 499 "Modeling Bacterial Growth." Spring 2012, Fall 2012.

30. Seung Yun Song. MSE 499 "Textured Piezoelectrics." Spring 2013. Fall 2013, Spring 2014, Fall 2014, Spring 2015.

31. Michael Ju. MSE 499 "Battery Modeling." Spring 2013.

32. Derek Shih. MSE 499 "Battery Model." Fall 2013.

33. Huaixun Hu Yan MSE 499 "Tortuosity Design." Fall 2013, Spring 2014.

34. Joe Carabetta. MSE 499 "Nanodot Based Batteries." Fall 2013, Spring 2014.

35. Jingyuan Liang "Kinetic Simulation Tool." SURF 2013.

36. Zaiwei Zhang. "VKML, version 2." SURF 2013, MSE 499 Spring 2014.

37. Derek Shih. MSE 499 "Electrochemical Shock Fracture." Spring 2014, Fall 2014, Spring 2015.

38. Drew Snook "Battery Undegraduate Research." MSE 499 Spring 2015, Fal 2015.

39. Ahmed Alghuraid "Battery Undergraduate Research." MSE 499 Spring 2015.

40. Ross Piedmonte "Undergraduate Battery Research." MSE 499 Spring 2015.

41. Lucas Robinson. "CAEBAT Battery Simulation." MSE 499 Spring 2015, SURF Summer 2015, MSE 499 Fall 2015. Spring 2016, Fall 2016, Spring 2017.

42. Adithya Bhattachar. "Simulation of Porous Battery." MSE 499 Spring 2015, Fall 2015.

43. Alvin Laimana. "Simulation of Grain Growth." MSE 499 Spring 2016.

44. Kaiyan Zhang "Battery Grain Boundaries." MSE 499. Fall 2016, Spring 2017.

45. Kevin Colbert "Fracture of Battery Materials." Fall 2016, Spring 2017.

46. Catherine Irwin "Electrochemical Modeling of Wulff Shapes." Spring 2019.

4.9 Short Courses and Workshops

1. Second Object Oriented Finite Element (OOF) Workshop (one day). NIST, June 2001, ~50 participants. Nature of Participation: Contributed with Lecture "*"Piezoelectricity and Beyond."*

2. Third Object Oriented Finite Element (OOF) Workshop (one day). NIST, August 2006, ~50 participants. Nature of Participation: Contributed with Lecture on "*OOF Extensions and Applications to Multifunctional Materials and Devices: An Overview."*

3. Object Oriented Finite Element (OOF)2/Toyota Workshop: Introduction to Modeling of Piezoelectric Microstructures. (one day). Purdue University, January 2009, 4 participants. Nature of Participation: Organized entire agenda and introduced the Object Oriented Finite Element Analysis program, reviewed the Finite Element method and taught numerical techniques to analyze two-dimensional piezoelectric microstructures.

4. Batteries Toyota Workshop. Purdue University, November 20, 2009, 6 participants. Nature of Participation: Presented challenges and opportunities in rechargeable battery technology.

5. Piezos3D Workshop (two days). Nagoya, Japan, June 8 and 9, 2010, 6 participants. Nature of Participation: Organized entire agenda and introduced the Toyota-sponsored and recently developed Piezos3D software and associated libraries. *Day 1:* Basic elements of numerical modeling, convergence, stability and discretization of 3D mathematical problem. *Day 2:* 3D polycrystalline piezoelectric modeling, visualization, and extension of the program. Performed advanced exercises to simulate complex three-dimensional electromechanical solids.

6. ICME Workshop (two weeks, June 2011, June 2012, June 2013, June 2016, June 2017). To address the educational challenges in integrating the complexity of the physics and multiscale nature of materials, the "Summer School for Integrated Computational Materials Education," was developed as a two-week program that includes a "crash course" on

computational materials science and engineering (CMSE) and focus sessions on educational modules that can be adopted into existing core courses. Tools into undergraduate-level thermodynamics, kinetics, material physics, and mechanical behavior courses.

5 Media

1. *"Introducing New Faculty."* **Impact Magazine,** Fall 2005*, pg. 1.*

2. *"Fuel Cell Success Hinges on Materials Engineers."* **Impact Magazine,** *Fall 2005, pgs. 5-6.*

3. *"Influence of Grain Boundaries on Ferroelectric Domain Hysteresis"* B. Huey,* R. E. García, and J. E. Blendell. **JOM** (October 2006).

4. *"Around MSE. Q&A with R. Edwin García. Considering Computational Materials Engineering."* **Impact Magazine,** Summer 2008, pgs. 2-3.

5. "Aperture: Central Page Inset." **Impact Magazine,** Summer 2008, pg. 12.

6. *"Computational Materials Science and Engineering Education: A Survey of Trends and Needs."* K. Thornton,* S. Nola,* R. E. García,* M. Asta,* and G.B. Olson. **JOM**, October, 2009.

7. *"Freeing Gallium Nitride Nanorods from Dislocations."* **Spotlights, School of Materials Engineering Web Page**, May 2010. (old link here, might not open).

8. "DOE Computational Science and Chemistry for Innovation Workshop." Final report Future Directions of Example Application and Innovation Contribution. R. E. García and Z. Liang. October, 2010. See inset on page 18 of final report.
http://www.ornl.gov/sci/cmsinn/CMSC_Workshop_Report.pdf

9. Spotlight Highlighting Ding-Wen (Tony) Chung's contribution to Nature Nanotechnology paper. Purdue Materials Engineering Web Page: old link here, might not open

10. ORNL Press Release Highlighting Purdue University contribution (with Senior MSE Tony Chung) to Nature Nanotechnology Paper WebPage: old link here, might not open

11. "Analytical theory may bring improvements to lithium-ion batteries." Writer: Emil Venere, 765-494-4709, venere@purdue.edu.
https://www.purdue.edu/newsroom/releases/2013/Q1/ March 5, 2013.
http://analytical-theory-may-bring-improvements-to-lithium-ion-batteries.html

12. "Dendrite Suppression to Curtail Lithium-Ion Battery Failure."
old link here, might not open

13. "Study Shows How to Stop Lithium Dendrite Formation in Batteries." Ovidiu Sandru March 9, 2013. old link here, might not open

14. "Suppressing Dendrite Growth Can Reduce Failure of Lithium Batteries." Laurie's Blog. June 22, 2013. old link here, might not open

15. "Study Shows How To Stop Lithium Dendrite Formation In Batteries." Ovidiu Sandru 2013-3-13. http://en.escn.com.cn/article/show/9667.aspx

16. "Analytical Theory Could Improve Lithium-Ion Batteries." Bob Michaels, March 11, 2013. old link here, might not open

17. "THEORETICAL ELIMINATION OF LITHIUM-ION DENDRITES DISCOVERED." Mar 06, 2013. old link here, might not open

18. "Analytical theory may bring improvements to lithium-ion batteries." Emil Venere. 03/05/2013. old link here, might not open

19. "Eliminating dendrite formation." Ruth Williams, 17 April 2013.
http://bestmag.co.uk/shop/news/042013-397/#.Uy0Eh9w6LPY

20. “Analytical theory may bring improvements to lithium-ion batteries.” Emil Venere. 5-Mar-2013. old link here, might not open

21. “How lithium electrochemical research might save the Boeing Dreamliner.” George Koprowicz, March 6, 2013. old link here, might not open

22. “Why It Takes So Long to Charge Your Devices — For Now.” Jim Nash, April 25 2013. old link here, might not open

23. “Purdue researchers aim to improve battery life | WLFI.” 2013.
old link here, might not open

24. “Analytical theory may bring improvements to lithium-ion batteries.” Purdue Alumnus May/June 2013. Pg. 44. old link here, might not open

25. “Research aims to improve lithium-based batteries.” January 2015.
old link here, might not open

26. “Improved dendrite formation control helps lithium batteries last longer.” January 2015. old link here, might not open

27. “Research to Bring Innovation to Lithium-based Batteries.” January 2015.
old link here, might not open

28. “Research aims to improve lithium-based batteries.” January 2015.
old link here, might not open

29. “Development in Lithium-Ion Batteries.” January 2015.
old link here, might not open

30. “Research aims to improve lithium-based batteries.” January 2015.
link here, might not open

31. “Materials study probes ’field-assisted’ processing for high-tech ceramic components.” January 24, 2017. link here; might change location

32. “Multi-University effort will advance materials, define the future of mobility.” April 3rd, 2017. link here; might change location

33. “Joint Research Initiative are Defining Autonomous Cars.” April 5th, 2017.
link here; might change location

34. “‘Data-driven’ design could lead to improved lithium-ion batteries.” April 24, 2017. link here; might change location

35. “Taming ‘dendrites’ could bring better lithium-ion batteries.” November 7, 2017. link here; might change location

36. Taming ‘dendrites’ could bring better lithium-ion batteries.” November 7, 2017. https://techxplore.com/news/2017-11-dendrites-lithium-ion-batteries.html

37. Taming ‘dendrites’ could bring better lithium-ion batteries.” November 7, 2017. https://www.nanowerk.com/nanotechnology-news/newsid=48568.php