

# Curriculum Vitae

## ASEGUN HENRY

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Assistant Professor  
Woodruff School of Mechanical Engineering  
School of Materials Science and Engineering  
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### RESEARCH INTERESTS

Utility scale renewable energy technology development, concentrated solar thermochemical energy conversion and reactor design; Concentrated solar thermal energy conversion and high temperature receiver design; Experimental and theoretical modeling of high temperature material/thermodynamic properties; High temperature thermal storage and thermochemical energy storage; Atomistic level modeling to study nanoscale energy and transport, phonon transport in bulk materials and at interfaces, high thermal conductivity polymers and ceramics; Molecular dynamics, first principles modeling, density functional theory.

### EDUCATION

2006 – 2009



**Massachusetts Institute of Technology**

**Ph.D. in Mechanical Engineering**

Thesis committee: Gang Chen (Advisor)

Mildred Dresselhaus, John Lienhard

Ph.D. Thesis: “1D-to-3D Transition of Phonon Heat Conduction in Polyethylene Chains Using Molecular Dynamics Simulations”

2004 – 2006



**M.S. in Mechanical Engineering**

Thesis Advisor: Gang Chen

Masters Thesis: “Molecular Dynamics Analysis of Spectral Characteristics of Phonon Heat Conduction in Silicon”

2000 – 2004



**Florida Agricultural & Mechanical University**

**B.S. in Mechanical Engineering, *summa cum laude***

Advisor: Makola Abdullah

Research: Developed numerical models for the dynamics of structural vibration during earthquakes.

## PROFESSIONAL EXPERIENCE

2012 – Present



**George W. Woodruff School of Mechanical Engineering**  
**School of Materials Science and Engineering**  
**Georgia Institute of Technology, Atlanta, GA**  
**Assistant Professor**

**PI - Atomistic Simulation & Energy (ASE) Research Group**

Current research topics include: High temperature concentrated solar power (CSP) receiver design using liquid metal heat transfer fluids; Oxygen storage material design and testing for high temperature solar thermochemical reactors, using DFT and high temperature TGA measurements; Solar thermochemical reactor design, modeling and optimization; Design and development of high thermal conductivity materials – polymers & high temperature ceramics; Molecular dynamics simulations of single polymer chains and bulk crystals; Thermal interface resistance modeling and theoretical development using equilibrium molecular dynamics simulations and DFT calculations.



2011 – 2012



**Advanced Research Projects Agency – Energy (ARPA-E)**  
**U.S. Department of Energy, Washington, D.C.**

**Fellow**

Developed new high risk/high reward ideas and concepts for potential funding opportunity announcements. Conducted due diligence, organized and hosted workshops on the agency's emerging ideas – i.e. heat engines with no moving parts as topping cycles for more efficient utility scale energy conversion & advanced spectral splitting optics for higher efficiency concentrated photovoltaics. Several ideas developed went on to seed the \$30M Full-Spectrum Optimized Conversion and Utilization of Sunlight (FOCUS) program, which was centered on concentrated solar technologies.

2010 – 2011



**Department of Material Science**  
**Northwestern University, Evanston, IL**

**Chris Wolverton, PI**

**Visiting Scholar/Postdoctoral Researcher**

Used first principles electronic structure calculations (DFT+U) to design and evaluate the thermodynamic properties of ceria alloys ( $\text{Ce}_{1-x-y}\text{Zr}_x\text{Ti}_y\text{O}_{2-\delta}$ ) for use in solar driven high temperature thermochemical water splitting reactors.

2009 – 2010



**Materials Theory Group**

**Oak Ridge National Laboratory, Oak Ridge, TN**

**David Singh, PI**

**Postdoctoral Researcher**

Theoretical development and implementation of a first principles method for calculating thermal conductivity. First principles prediction of a morphotropic phase boundary in bismuth based perovskite ferroelectrics.

2004 – 2009



**NanoEngineering Group**

**Department of Mechanical Engineering**

**MIT, Cambridge, MA**

**Professor Gang Chen, PI**

**Graduate Research Assistant**

Developed codes for parallel molecular dynamics simulations and lattice dynamics calculations. Conducted detailed analysis of phonon transport (spectral dependence) in bulk silicon. Conducted detailed analyses of phonon transport in one-dimensional conductors, such as polyethylene chains and carbon nanotubes.

Summer 2006



**Sandia National Laboratories, Albuquerque, NM**

**Dr. Steven Plimpton**

**Graduate Research Assistant**

Implemented the adaptive intermolecular empirical bond order potential (AIREBO) for hydrocarbon systems, into the large atomic/molecular massively parallel simulator (LAMMPS).

Summer 2004



**NanoEngineering Group**

**Department of Mechanical Engineering**

**MIT, Cambridge, MA**

**Professor Gang Chen, PI**

**Research Assistant**

Developed code for calculating the thermal conductivity of solid argon using molecular dynamics simulations.

Summer 2003



**NanoEngineering Group**

**Department of Mechanical Engineering**

**MIT, Cambridge, MA**

**Professor Gang Chen, PI**

**Research Assistant**

Developed a numerical modeling scheme for experimentally determining the thermoelectric properties of thin films, when temperature measurements are absent.

Summer 2002



**The University of Tokyo, Tokyo Japan**

**Research Experiences for Undergraduates in Japan in Advanced Technology (REUJAT)**

**Professor Makola Abdullah, PI**

**Research Assistant**

Invented, designed and modeled the structural magnetic induction damper (SMID), a new type of passive device for reducing structural vibration during earthquakes while simultaneously storing the energy as electricity.

Summer 2001



**Visteon Automotive, Ypsilanti, MI**

**Alternator Division Intern**

Alternator voltage regulator failure analysis test box development. 6<sup>th</sup> Generation Integrated Regulator Rectifier (IRR) alternator product testing, design, modification and development.

## AWARDS AND HONORS

2010-2011	Ford Foundation Postdoctoral Fellowship  FORDFOUNDATION
2009-2010	UNCF-MERCK Postdoctoral Fellowship  UNCF
2005-2009	DOE – Computational Science Graduate Fellowship  DOE CSGF
2005-2006	MIT Black Graduate Students Association – Community Service Award
2004-2005	MIT – Lemelson Presidential Fellowship 
2000-2004	FAMU – Distinguished Scholars Award  FAMU <small>FLORENCE ROBERTS COLLEGE OF ENGINEERING AND MECHANICAL UNIVERSITY</small>
2002-2004	FAMU – Pi Tau Sigma Mechanical Engineering Society
2001-2004	FAMU – Tau Beta Pi Engineering Honors Society

## JOURNAL PUBLICATIONS

- [1] A. Henry and G. Chen, *Spectral Phonon Transport Properties of Silicon Based on Molecular Dynamics Simulations and Lattice Dynamics*, J. Comput. Theor. Nanosci., 5, 141-152 (2008). - [Over 220 citations – Google Scholar]

- [2] A. Henry and G. Chen, *High Thermal Conductivity of Single Polyethylene Chains Using Molecular Dynamics Simulations*, **Phys. Rev. Lett.**, 101, 235502 (2008). - [Over 90 citations – Google Scholar]
- [3] A. Henry and G. Chen, *Anomalous heat conduction in polyethylene chains: Theory and molecular dynamics simulations*, **Phys. Rev. B**, 79, 144305 (2009). - [Over 50 citations – Google Scholar]
- [4] A. Henry and G. Chen, *Explicit Treatment of Hydrogen in Thermal Simulations of Polyethylene*, **J. Nanoscale and Microscale Thermophysical Engineering**, 13, 2, 99-108 (2009).
- [5] M. S. Dresselhaus, G. Chen, Z. F. Ren, G. Dresselhaus, A. Henry, J.-P. Fleurial, *New Composite Thermoelectric Materials for Energy Harvesting Applications*, **JOM**, 61, 4, 86 (2009).
- [6] S. Shen, A. Henry, J. Tong, R. Zheng, G. Chen, *Polyethylene nanofibres with very high thermal conductivities*, **Nature Nanotechnology**, 5, 251 - 255 (2010) - [Over 130 citations – Google Scholar]
- [7] V. R. Cooper, A. Henry, S. Takagi, D. J. Singh, *First principles prediction of a morphotropic phase boundary in the  $Bi(Zn_{1/2}Ti_{1/2})O_3-(Bi_{1/2}Sr_{1/2})(Zn_{1/2}Nb_{1/2})O_3$  alloy*, **Appl. Phys. Lett.**, 98, 122903 (2011).
- [8] T. Luo, K. Esfarjani, J. Shiomi, A. Henry, and G. Chen, *Molecular dynamics simulation of thermal energy transport in polydimethylsiloxane*, **Journal of Applied Physics**, 109, 074321-1-6 (2011).
- [9] Z. Tian, K. Esfarjani, J. Shiomi, A. Henry, G. Chen, *On the importance of optical phonons to thermal conductivity in nanostructures*, **Applied Physics Letters**, 99, 053122-1-3 (2011).
- [10] Y. Chalopin, K. Esfarjani, A. Henry, S. Volz, and G. Chen, *Thermal interface conductance in Si/Ge superlattices by equilibrium molecular dynamics*, **Phys. Rev. B** 85, 195302 (2012).
- [11] N. Yang, T. Luo, K. Esfarjani, A. Henry, Z. Tian, J. Shiomi, Y. Chalopin, B. Li, G. Chen, *Thermal Interface Conductance between Aluminum and Silicon by Molecular Dynamics Simulations*, **J. Comput. Theor. Nanosci.**, In Press (2014).
- [12] V. Singh, T. L. Bougher, A. Weathers, Y. Cai, K. Bi, M. T. Pettes, S. A. McMEnamin, W. Lv, D. P. Resler, T. R. Gattuso, D. H. Altman, K. H. Sandhage, L. Shi, A. Henry and

B. A. Cola, High Thermal Conductivity of Chain-Oriented Amorphous Polythiophene, *Nature Nanotechnology*, 9, 384-390 (2014).

[13] A. Henry, R. Prasher, The Prospect of Solid State Energy Conversion to Reduce the Cost of Concentrated Solar Power, **Energy & Environmental Science**, 7, 1819-1828 (2014).

[14] K. Gordiz, A. Henry, New Insights Into Phonon Transport at Interfaces, *Nature Communications*, In Review.

[15] W. Lv, A. Henry, Theoretical Prediction of Room Temperature Thermal Superconductivity in Polythiophene, *Scientific Reports*, In Review.

[16] [17] C. Yuan, Y. Kawajiri, W. Chueh, C. Jarrett, K. Sandhage A. Henry, A New High Efficiency Solar Fuels Reactor Concept Based on a Liquid Metal Heat Transfer Fluid: Modeling and Efficiency Estimation, *Applied Energy*, In Review.

[17] C. Jarrett, W. Chueh, Y. Kawajiri, C. Yuan, K. Sandhage, A. Henry, Critical Limitations on the Efficiency of Two-Step Thermochemical Cycles, *Applied Energy*, In Review.

## INVITED BOOK CHAPTERS

[1] A. Henry, *Thermal Transport in Polymers*, Invited chapter in the Annual Review of Heat Transfer, In Press (2013). DOI: 10.1615/AnnualRevHeatTransfer.2013006949

## CONFERENCE PUBLICATIONS

[1] A. Henry and G. Chen, *Thermal Conductivity of Polyethylene Chains Using Molecular Dynamics Simulations*. published in the Proceedings of the 3<sup>rd</sup> Energy Nanotechnology International Conference, 2008. Jacksonville, Florida USA.

[2] A. Henry and G. Chen, *Normal Mode Analysis of Single Polyethylene Chains*. published in the Proceedings of the ASME International Mechanical Engineering Congress and Exposition. 2008. Boston, Massachusetts USA.

[3] A. Henry and G. Chen, *Analysis of Heat Conduction in Silicon Using Molecular Dynamics Simulations*. published in the Proceedings of the ASME International Mechanical Engineering Congress and Exposition. 2006. Chicago, Illinois USA.

- [4] A. Henry, A. Richardson and M. Abdullah, published in SEMS 2001: International Conference on Structural Engineering, Mechanics and Computation, 2, 887-895 (2001).

## OTHER PUBLICATIONS

- [1] G. Chen, S. Shen, A. Henry, J. Tong, *Heat Conducting Polymers*, Materials World Magazine, 18, 23-25 (2010).
- [2] G. Chen, S. Shen, J. Tong, A. Henry, *Reinventing the Polymer*, The Chemical Engineer, 827, 28-29 (2010).

## CONFERENCE PRESENTATIONS

- [1] A. Henry and G. Chen, *High Thermal Conductivity of Polyethylene Chains Using Molecular Dynamics Simulations*. 3<sup>rd</sup> Energy Nanotechnology International Conference, 2008. Jacksonville, Florida USA.
- [2] A. Henry and G. Chen, *High Thermal Conductivity of Polyethylene Using Molecular Dynamics Simulations*. 6th US-Japan Joint Seminar on Nanoscale Transport Phenomena, 2008. Boston MA USA.
- [3] A. Henry and G. Chen, *Thermal Conductivity of Single Polyethylene Chains Using Molecular Dynamics Simulations*. DOE Computational Science Graduate Fellows Conference, 2008. Washington D.C. USA.
- [4] A. Henry, G. Chen and S. Plimpton, *Molecular Dynamics Simulations of MWCNTs and Polyethylene Chains Using Molecular Dynamics*. DOE Computational Science Graduate Fellows Conference, 2007. Washington D.C. USA.
- [5] A. Henry and G. Chen, *Analysis of Heat Conduction Using Molecular Dynamics Simulations*. DOE Computational Science Graduate Fellows Conference, 2006. Washington D.C. USA.
- [6] A. Henry and G. Chen, *Analysis of Heat Conduction in Silicon Using Molecular Dynamics Simulations*. IMECE, 2006. Chicago, IL USA.
- [7] A. Henry and M. Abdullah, *Structural Magnetic Induction Damper*, Japan Society for the Promotion of Science, Symposium on Structural Control and Health Monitoring, 2002. Tokyo, Japan.

- [8] A. Henry, M. Abdullah, *Structural Magnetic Induction Damper*, FAMU Undergraduate Program UROP Technical Research Symposium, 2002. Tallahassee, FL USA -- *1<sup>st</sup> Place Presentation Award*.
- [9] A. Henry, A. Richardson and M. Abdullah, *Placement and Elimination of Vibration Controllers in Tall Buildings*, Undergraduate Students in Technical Research (USTR) competition, NSBE national convention 2001. Indianapolis, IN USA.
- [10] A. Henry, A. Richardson and M. Abdullah, *Placement and Elimination of Vibration Controllers in Tall Buildings*, Universidad Metropolitana Undergraduate Research Science Symposium, 2000. San Juan Puerto Rico.
- [11] K. Gordiz and A. Henry, *Ensemble Averaging vs. Time Sampling for Molecular Dynamics Simulations of Thermal Conductivity*, 11th AIAA/ASME Joint Thermophysics and Heat Transfer Conference. 2014. Atlanta, GA USA.
- [12] K. Gordiz and A. Henry, *Modal Decomposition of Thermal Transport Across Interfaces*, 11th AIAA/ASME Joint Thermophysics and Heat Transfer Conference, 2014. Atlanta, GA USA.
- [13] C. Jarrett, A. Henry, *Screening of Oxides for Solar Driven Thermochemical Water Splitting*, 11th AIAA/ASME Joint Thermophysics and Heat Transfer Conference, 2014. Atlanta, GA USA.
- [14] A. DeAngelis, A. Henry, *Sensitivity Analysis of a High Temperature Liquid Metal Based Solar Receiver*, 11th AIAA/ASME Joint Thermophysics and heat Transfer Conference, 2014. Atlanta, GA USA.
- [15] W. Lv, A. Henry, *Molecular Dynamics Simulations of Thermal Transport in Single Polythiophene Chains*, 11th AIAA/ASME Joint Thermophysics and Heat Transfer Conference, 2014 Atlanta, GA USA.
- [16] W. Lv, A. Henry, *Spectral Phonon Transport Properties from Direct Green-Kubo Thermal Conductivity Decomposition*, 11th AIAA/ASME Joint Thermophysics and Heat Transfer Conference, 2014. Atlanta, GA USA.
- [17] G. Wilk, A. Henry, *Radiation Heat Sink for Heat Dissipation in Liquid Metal Loops*, 11th AIAA/ASME Joint Thermophysics and Heat Transfer Conference, 2014. Atlanta, GA USA.



- [18] A. Henry, *A New Reactor Concept for Two-Step Solar Thermochemical Energy Conversion Using a Liquid Metal Heat Transfer Fluid*, ASME Conference on Energy Sustainability, 2014. Boston MA USA.
- [19] A. Henry, *High Temperature Concentrated Solar Power Using a Liquid Metal Heat Transfer Fluid*, ASME Conference on Energy Sustainability, 2014. Boston MA USA.

## INVITED SEMINARS

### *“Phonon Transport in Polyethylene Using Molecular Dynamics Simulations”*

- [1] Northeastern University, Department of Mechanical Engineering – December 2008
- [2] Georgia Institute of Technology, Department of Mechanical Engineering – February 2009
- [3] Oak Ridge National Laboratories, Division of Computational Science – March 2009
- [4] Vanderbilt University, Department of Mechanical Engineering – March 2009
- [5] University of California Berkeley, Department of Mechanical Engineering – March 2009
- [6] Lawrence Livermore National Laboratories, Quantum Simulation Group – March 2009
- [7] Stanford University, Department of Material Science – April 2009

## PATENTS AND DISCLOSURES

- [1] 2014 Utility Patent Application, Concentrated Solar Thermophotovoltaics with Storage
- [2] 2013 Provisional Patent Application, Concentrated Solar Thermophotovoltaics with Storage
- [3] 2013 Utility Patent Continuation 13/538,304, “Solar Receivers for Use in Solar-Driven Thermochemical Processes”, In Review.
- [4] 2012 Utility Patent Application 13/538,304, “Reactor, System and Method for Solid Reactant Based Thermochemical Processes”, In Review.

## PROFESSIONAL ACTIVITIES

### **Journal Referee for:**

Physical Review Letters  
Physical Review B  
Applied Physics Letters  
Computational Materials Science  
Journal of Applied Physics  
Journal of Chemical Physics  
Journal of Physical Chemistry B  
European Physical Journal  
ASME Journal of Heat Transfer  
Journal of CO<sub>2</sub> Utilization  
Journal of Solar Energy Engineering  
Nano Letters

**Proposal Referee for:**

National Science Foundation – Scalable Nano-Manufacturing  
Department of Energy – SunShot CSP

**Societal Memberships:**

American Society of Mechanical Engineers  
ASME K-9 Nanoscale Thermal Transport Committee  
American Physical Society  
American Ceramic Society  
National Society of Black Engineers

**Service:**

2012-Present ASME Nanoscale Thermal Transport Division Committee Member  
2013 Solar PACES – Thermal Receivers Session Chair  
2013 IMECE – Nanoparticles and Nanofluids Session Chair

**FUNDED PROJECTS**

**Source: Advanced Research Projects Agency – Energy (ARPA-E)**

**Project Title: High Efficiency Solar Fuels Reactor Concept**

**Award Size: \$3,549,490**

Performance Period: April 2013-April 2016

Program Manager: Howard Branz

PI: Asegun Henry

Co-PIs: Kenneth Sandhage (Georgia Institute of Technology), Yoshiaki Kawajiri (Georgia Institute of Technology), William Chueh (Stanford University), Duncan Moore (University of Rochester).

**Source: Intel Corp.**

**Project Title: High Thermal Conductivity Polymer Composites for Improved Heat Dissipation in Electronic Packages**

**Award Size: \$323,217**

Performance Period: April 2013-April 2016

Program Manager: Mondira Pant

PI: Asegun Henry

Co-PIs: Kyriaki Kalaitzidou