Alan McGaughey

Trustee Professor of Mechanical Engineering
Carnegie Mellon University
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Nanoscale Transport Phenomena Laboratory

Professional Experience

Carnegie Mellon University, Pittsburgh, PA, August 2005 -

- Department of Mechanical Engineering: Trustee Professor (2021-) Professor (2014-2021), Associate Professor (2010-2014), Assistant Professor (2005-2010)
- Department of Materials Science and Engineering (courtesy appointment)

University of Florida, Gainesville, FL, August 2004-July 2005

- Post-doctoral fellow in the Department of Materials Science and Engineering. Advisors: Professors S. R. Phillpot, S. B. Sinnott, and J. C. Yang (University of Pittsburgh).

Education

University of Michigan, Ann Arbor, Michigan, September 2000-June 2004

- Ph.D. Thesis: "Phonon transport in molecular dynamics simulations: Formulation and thermal conductivity prediction." Advisor: Professor M. Kaviany, Department of Mechanical Engineering.

University of Toronto, Toronto, Ontario, September 1998-August 2000

- Master of Applied Science. Thesis: "The evaporation and stability of a droplet in a finite system." Advisor: Professor C. A. Ward, Department of Mechanical and Industrial Engineering.

McMaster University, Hamilton, Ontario, September 1994-April 1998

- Bachelor of Engineering, Department of Mechanical Engineering.

Awards

Research and Academics

- Fellow of the American Physical Society, 2021
- Viskanta Fellowship, Purdue University, 2021
- Trustee Professor of Mechanical Engineering, Carnegie Mellon University, 2021
- Invitational Fellowship for Research in Japan, Japan Society for the Promotion of Science, 2021 (declined due to COVID-19 pandemic)
- Fellow of the American Society of Mechanical Engineers, 2016
- American Physical Society Outstanding Referee, 2015
- Harrington Faculty Fellow, University of Texas at Austin, 2012-2013
- Air Force Office of Scientific Research Young Investigator Program, 2009
- University of Michigan Rackham School of Graduate Studies Distinguished Dissertation Award, 2004.
- University of Michigan Rackham School of Graduate Studies Pre-Doctoral Fellowship, 2003-2004
- University of Michigan College of Engineering Distinguished Achievement Award, Department of Mechanical Engineering, 2003 and 2004
- Natural Sciences and Engineering Research Council of Canada Postgraduate Studies B Scholarship (NSERC PGSB), held May 2001-April 2003 at the University of Michigan
- NSERC PGSA, held September 1998-August 2000 at the University of Toronto
- Association of Professional Engineers Gold Medal, McMaster University, May 1998: Highest cumulative average in graduating engineering class ($\sim$400).
- The Iroquois Trophy, McMaster University, May 1998: Highest cumulative average in graduating mechanical engineering class ($\sim$80).
- Canada Scholars Special Corporate Award: Atomic Energy of Canada Limited (AECL) Award, McMaster University, 1997
- Canada Scholarship, held September 1994-April 1998 at McMaster University

Teaching and Service

- Philip L. Dowd Fellowship, Carnegie Mellon University, 2019
- Professor of the Year, Mechanical Engineering, Carnegie Mellon University, 2012, 2015, and 2017 (voted by graduating seniors)
- National Academy of Engineering, Frontiers of Engineering Education Symposium, 2015
- Benjamin Richard Teare Teaching Award, Carnegie Mellon University, 2014
- Struminger Junior Faculty Fellow, Carnegie Mellon University, 2009
- University of Michigan College of Engineering Distinguished Leadership Award, 2004
- Outstanding Graduate Student Instructor Award, University of Michigan, April 2002

Supervision

Post-doctoral fellows: Haibin Chen (2009-2011), Joe Turney (2010)*, Minyoung Lee (2011), Lin Hu (2011-2012), Hasan Babaei+ (2015-2018), Abhishek Pathak# (2023-), Manoj Settipalli (2023-). Co-advised with: * Cristina Amon, + Chris Wilmer, # Jonathan Malen.

Ph.D. students: Eric Landry (2007-2009), Joe Turney* (2006-2009), John Thomas (2006-2010), Minyoung Lee (2006-2010), Jason Larkin (2009-2013), Wee-Liat Ong+ (2010-2014), Ankit Jain (2011-2015), Shubhaditya Majumdar+ (2011-2016), Ivy Yu (2011-2016), Simon Lu (2011-2016), Francisco Ramirez (2015-2017), Kevin Parrish+ (2013-2017), Henry Aller+ (2016-2021), Hyun-Young Kim (2016-2021), Xiaoman Wang+ (2017-2021), Jie Gong (2017-2022), Holden Parks# (2017-2022), Shuyan Zhang& (2018-2022), Hariharan Ramasubramanian (2021-), Ethan Meitz (2022-)%, Nathan Wasserman (2022-)@. Co-advised with: * Cristina Amon, + Jonathan Malen, # Venkat Viswanathan, & Reeja Jayan, % Gerald Wang, @ Sneha Parra.

Masters students: Eric Landry (2005-2007), Alex Massicotte (2010-2013), Kevin Parrish (2012-2013), Matthew McIntosh (2013-2015), Caroline Gorham (2014-2015), Paarth Thapur (2015-2016), Sushant Kumar (2015-2017), Matthew Bartnof+ (2017-2019), Jinchen Han (2018-2019), Yang Li (2018-2020), Niranjan Bhombe (2022-).

Undergraduate students: Sarat Mikkilineni (2006), Madhur Paharia (2006-2007), Takahiro Matsuura (2007), Gary Lee (2007, 2009-2010), Chris Fleck (2008-2010), Ottoleo Kuter-Arnebeck (2008-2009), Nicholas Roche (2008-2009), Ryan Iutzi (2009), Shaun Swanson (2009-2010), Lucian Cesca (2009), Michael Barako (2009-2010), Gabriella Coloyan (2010-2012), Melanie Jasper (2012), Alex Kowalski (2012), Josh Fuhrman (2014-2015), Justin Abel (2015-2016), Andy Birla (2016-2017), James Zhang (2017), Evan Larrick (2017), Lane Darby (2019), Aaron McKenzie (2019), Rohan Mehta (2020), Michael Pang (2021), Ivy He

(2021), Sharon Chu (2021-2022), Daniel Xiao (2020-2023), Michael Rapp (2023-).

Visitors: Ryan Iutzi (2009), Dan Sellan (2009), Yusuke Masao (2012), Sam Huberman (2012), Kimmo Saaskilahti (2015), Cheng Shao (2016-2017), I-Ling Chang (2017), Bo Fu (2018-2019), Qi Liang (2019), Jiong Chen (2020).

Contributions to Research

Google Scholar. Citations: 12,230, h-index: 54 (08/08/23)

Book Chapters and Review Articles

4. F. DeAngelis, M. G. Muraleedharan, J. Moon, H. R. Seyf, A. J. Minnich, A. J. H. McGaughey, and A. Henry, "Thermal transport in disordered materials." *Nanoscale and Microscale Thermophysical Engineering* **23**, 81-116 (2019).

3. A. J. H. McGaughey, A. Jain, H.-Y. Kim, and B. Fu, "Phonon properties and thermal conductivity from first principles, lattice dynamics, and the Boltzmann transport equation." *Journal of Applied Physics* **125**, 011101 (2019). **Featured Article.**

2. A. J. H. McGaughey and J. M. Larkin, "Predicting phonon properties from equilibrium molecular dynamics simulations." *Annual Review of Heat Transfer Volume 17*, 49-87 (Begell House, 2014).

1. A. J. H. McGaughey and M. Kaviany, "Phonon transport in molecular dynamics simulations: Formulation and thermal conductivity prediction." *Advances in Heat Transfer Volume 39*, 169-255 (Academic Press, 2006).

Journal Publications

106. L. Su, S. Zhang, A. J. H. McGaughey, B. R. Jayan, and A. Manthiram, "Battery charge curve prediction via feature extraction and supervised machine learning." To appear in *Advanced Science.*

105. M.Islamov, P. Boone, H. Babaei, A. J. H. McGaughey, and C. E. Wilmer, "Correlated missing linker defects increase thermal conductivity in metal-organic framework UiO-66." *Chemical Science* **14**, 6592 (2023).

104. S. Zhang, J. Gong, S. Chu, D. Z. Xiao, B. R. Jayan, and A. J. H. McGaughey, "Pair distribution function analysis for oxide defect identification through feature extraction and supervised learning." *APL Machine Learning* **1**, 026115 (2023).

103. M. Islamov, H. Babaei, R. Anderson, K. B. Sezginel, J. R. Long, A. J. H. McGaughey, D. A. Gomez-Gualdron, and C. E. Wilmer. "High-throughput screening of hypothetical metal-organic frameworks for thermal conductivity." *npj Computational Materials* **9**, 11 (2023).

102. S. Zhang, J. Gong, D. Xiao, B. R. Jayan, and A. J. H. McGaughey, "Pair distribution function analysis driven by atomistic simulations: Application to microwave radiation synthesized TiO_2 and ZrO_2." *Computational Materials Science* **218**, 111964 (2023).

101. X. Wang, S. A. Ghaffarizadeh, X. He, A. J. H. McGaughey, and J. A. Malen, "Ultrahigh evaporative heat transfer measured locally in submicron water films." *Scientific Reports* **22**, 22353 (2022).

100. J. J. Wang, J. Gong, A. J. H. McGaughey, and D. Segal, "Simulations of heat transport in single-molecule junctions: Investigations of the thermal diode effect." *Journal of Chemical Physics* **157**, 174105 (2022).

99. J. Gong, S. Chu, R. Mehta, and A. J. H. McGaughey, "XGBoost model for electrocaloric temperature change predictions in ceramics." *npj Computational Materials* **8**, 140 (2022).

98. M. E. DeCoster, H. Babaei, S. S. Jung, Z. Hassan, J. T. Gaskins, A. Giri, E. J. Tiernan, J. A. Tomko, H. Baumgart, P. M. Norris, A. J. H. McGaughey, C. E. Wilmer, E. Redel, A. Giri, and P. E. Hopkins, "Hybridization from guest-host interactions reduces the thermal conductivity of metal organic frameworks." *Journal of the American Chemical Society* **144**, 3603 (2022).

97. A. Giri, A. Evans, M. Rahman, A. J. H. McGaughey, and P. E. Hopkins, "Highly negative Poisson's ratio in thermally conductive covalent organic frameworks." *ACS Nano* **16**, 2843 (2022).

96. X. Wang, M. Jeong, A. J. H. McGaughey, and J. A. Malen, "Reducing the uncertainty caused by the laser spot radius in frequency-domain thermoreflectance measurements of thermal properties." *Review of Scientific Instruments* **93**, 023001 (2022).

95. B. Fu, G. Tang, and A. J. H. McGaughey, "Finite temperature force constants are essential for accurately predicting the thermal conductivity of rutile TiO_2." *Physical Review Materials* **6**, 015401 (2022).

94. H. T. Aller, J. A. Malen, and A. J. H. McGaughey, "Universal model for predicting the thermal boundary conductance of a multilayered-metal–dielectric interface." *Physical Review Applied* **15**, 064043 (2021). **Editor's Suggestion.**

93. A. M. Evans, A. Giri, V. K. Sangwan, S. Xun, M. Bartnof, C. G. Torres-Castanedo, H. B. Balch, M. S. Rahn, N. P. Bradshaw, E. Vitaku, D. W. Burke, H. Li, M. J. Bedzyk, F. Wang, J.-L. Brédas, J. A. Malen, A. J. H. McGaughey, M. C. Hersam, W. R. Dichtel, and P. E. Hopkins, "Thermally conductive ultra-low-k dielectric layers based on two-dimensional covalent organic frameworks." *Nature Materials* **20**, 1142 (2021).

92. C. Shao, W.-L. Ong, J. Shiomi, and A. J. H. McGaughey, "Nano-confinement between graphene walls suppresses the near-wall diffusion of the ionic liquid [BMIM][PF6]." *Journal of Physical Chemistry B* **125**, 4527-4535 (2021).

91. B. Smith, G. Coloyan Fleming, K. Parrish, F. Wen, E. Fleming, K. Jarvis, E. Tutuc, A. J. H. McGaughey, and L. Shi, "Mean free path suppression of low-frequency phonons in SiGe nanowires." *Nano Letters* **20**, 8384-8391 (2020).

90. Q. Liang, M. Bartnof, Y.-L. He, J. A. Malen, and A. J. H. McGaughey, "Fullerene rotational dynamics generate disordered configurations that suppress thermal conductivity in superatomic crystals." *Nanoscale Horizons* **5**, 1524-1529 (2020).

89. H. L. Parks, H.-Y. Kim, V. Viswanathan, and A. J. H. McGaughey, "Uncertainty quantification in first-principles predictions of phonon properties and lattice thermal conductivity." *Physical Review Materials* **4**, 083805 (2020).

88. H. Babaei, M. E. DeCoster, M. Jeong, Z. M. Hassan, T. Islamoglu, H. Baumgart, A. J. H. McGaughey, R. Engelbert, O. K. Farha, P. E. Hopkins, J. A. Malen, and C. E. Wilmer, "Observation of reduced thermal conductivity in a metal-organic framework due to the presence of adsorbates." *Nature Communications* **11**, 4010 (2020).

87. X. Wang, Y. Li, J. A. Malen, and A. J. H. McGaughey, "Assessing the impact of disjoining pressure on thin-film evaporation with atomistic simulation and kinetic theory." *Applied Physics Letters* **116**, 213701 (2020).

86. J. Gong and A. J. H. McGaughey, "Device-level thermodynamic model for an electrocaloric cooler." *International Journal of Energy Research* **44**, 5343 (2020).

85. B. Fu, K. D. Parrish, H.-Y. Kim, G. Tang, and A. J. H. McGaughey, "Phonon confinement and transport in ultrathin films." *Physical Review B* **101**, 045417 (2020).

84. H. T. Aller, X. Yu, A. Wise, R. Howell, A. J. Gellman, A. J. H. McGaughey, and J. A. Malen, "Chemical reactions impede thermal transport across metal/β-Ga_2O_3 interfaces." *Nano Letters* **19**, 8533-8538 (2019).

83. S. K. Jha, N. Nakamura, S. Zhang, L. Su, X. L. Phuah, H. Wang, H. Wang, J. S. Okasinski, A. J. H. McGaughey, B. Reeja-Jayan, "Defect-mediated anisotropic lattice expansion in ceramics as evidence for non-thermal coupling between electromagnetic fields and matter." *Advanced Engineering Materials* **21**, 1900762 (2019).

82. H.-Y. Kim, K. D. Parrish, and A. J. H. McGaughey, "Mapping phonon modes from reduced-dimensional to bulk systems." *Journal of Applied Physics* **126**, 144302 (2019).

81. H. L. Parks, A. J. H. McGaughey, and V. Viswanathan, "Uncertainty quantification in first-principles predictions of harmonic vibrational frequencies of molecules and molecular complexes." *Journal of Physical Chemistry C* **123**, 4072-4084 (2019).

80. E. S. O'Brien, J. C. Russell, M. Bartnof, A. D. Christodoulides, K. Lee, J. A. DeGayner, D. W. Paley, A. J. H. McGaughey, W.-L. Ong, J. A. Malen, X.-Y. Zhu, and X. Roy, "Spontaneous electronic band formation and switchable behaviors in a phase-rich superatomic crystal." *Journal of the American Chemical Society* **140**, 15601-15605 (2018).

79. S. Kumar, C. Shao, S. Lu, and A. J. H. McGaughey, "Contributions of different degrees of freedom to thermal transport in the C_{60} molecular crystal." *Physical Review B* **97**, 140303 (2018).

78. H. Babaei, A. J. H. McGaughey, and C. E. Wilmer, "Transient mass and thermal transport during methane adsorption into the metal-organic framework HKUST-1." *ACS Applied Materials & Interfaces* **10**, 2400-2406 (2018).

77. F. V. Ramirez, S. Shen, and A. J. H. McGaughey, "Near-field radiative heat transfer in graphene plasmonic nanodisk dimers." *Physical Review B* **96**, 165427 (2017).

76. F. V. Ramirez and A. J. H. McGaughey, "Plasmonic thermal transport in graphene nanodisk waveguides." *Physical Review B* **96**, 165428 (2017).

75. K. D. Parrish, J. R. Abel, A. Jain, J. R. Abel, J. A. Malen, and A. J. H. McGaughey, "Phonon-boundary scattering in nanoporous silicon films: Comparison of Monte Carlo techniques." *Journal of Applied Physics* **122**, 125101 (2017).

74. S. Lu and A. J. H. McGaughey, "Thermal conductance of graphene/hexagonal boron nitride heterostructures." *Journal of Applied Physics* **121**, 115103 (2017).

73. S. Majumdar, J. A. Malen, and A. J. H. McGaughey, "Cooperative molecular behavior enhances the thermal conductance of binary self-assembled monolayer junctions." *Nano Letters* **17**, 220-227 (2017).

72. H. Babaei, A. J. H. McGaughey, and C. E. Wilmer, "Effect of pore size and shape on the thermal conductivity of metal-organic frameworks." *Chemical Science* **8**, 583-589 (2017).

71. W.-L. Ong, E. O'Brien, P. Dougherty, D. Paley, C. F. Higgs III, A. J. H. McGaughey, J. A. Malen, and X. Roy, "Orientational order controls crystalline and amorphous thermal transport in superatomic crystals." *Nature Materials* **16**, 83-88 (2017).

70. K. Sääskilahti, J. Oksanen, J. Tulkki, A. J. H. McGaughey, and S. Volz, "Vibrational mean free paths and thermal conductivity of amorphous silicon from non-equilibrium molecular dynamics simulations." *AIP Advances* **6**, 121904 (2016).

69. R. Comin, M. K. Crawford, A. H. Said, N. Herron, W. E. Guise, X. Wang, P. S. Whitfield, A. Jain, X. Gong, A. J. H. McGaughey, and E. H. Sargent, "Lattice dynamics and the nature of structural transitions in organolead halide perovskites." *Physical Review B* **94**, 094301 (2016).

68. J. A. Sierra Suarez, S. Majumdar, A. J. H. McGaughey, J. A. Malen, and C. F. Higgs III, "Morse potential-based model for contacting composite rough surfaces: Formulation and application to self-assembled monolayer junctions." *Journal of Applied Physics* **119**, 145306 (2016).

67. A. Jain and A. J. H. McGaughey, "Thermal transport by phonons and electrons in aluminum, silver, and gold from first principles." *Physical Review B* **93**, 081206(R) (2016)

66. Y.-J. Yu and A. J. H. McGaughey, "Energy barriers for dipole moment flipping in PVDF-related ferroelectric polymers." *Journal of Chemical Physics* **144**, 014901 (2016).

65. Z. Liang, A. Jain, A. J. H. McGaughey, and P. Keblinski "Molecular simulations and lattice dynamics determination of Stillinger-Weber GaN thermal conductivity." *Journal of Applied Physics* **118**, 125104 (2015).

64. A. Jain and A. J. H. McGaughey, "Effect of exchange-correlation on first-principles-driven lattice thermal conductivity predictions of crystalline silicon." *Computational Materials Science* **110**, 115-120 (2015).

63. D. Li and A. J. H. McGaughey, "Phonon dynamics at surfaces and interfaces and its implications in energy transport in nanostructured materials - An opinion paper." *Nanoscale and Microscale Thermophysical Engineering* **19**, 166-182 (2015).

62. S. Majumdar, J. A. Sierra-Suarez, S. N. Schiffres, W.-L. Ong, C. F. Higgs III, A. J. H. McGaughey, and J. A. Malen, "Vibrational mismatch of metal leads controls thermal conductance of self-assembled monolayer junctions." *Nano Letters* **15**, 2985-2991 (2015).

61. S. Lu and A. J. H. McGaughey, "Thermal conductance of superlattice junctions." *AIP Advances* **5**, 053205 (2015).

60. A. Jain and A. J. H. McGaughey, "Strongly anisotropic in-plane thermal transport in single-layer black phosphorene." *Scientific Reports* **5**, 8501 (2015).

59. K. D. Parrish, A. Jain, J. M. Larkin, W. A. Saidi, and A. J. H. McGaughey, "Origins of thermal conductivity changes in strained crystals." *Physical Review B* **90**, 235201 (2014).

58. L. Hu and A. J. H. McGaughey, "Thermal conductance of the junction between single-walled carbon nanotubes." *Applied Physics Letters* **105**, 193104 (2014).

57. K. T. Regner, A. J. H. McGaughey, and J. A. Malen, "Analytical interpretation of non-diffusive phonon transport in thermoreflectance thermal conductivity measurements." *Physical Review B* **90**, 064302 (2014).

56. A. Jain and A. J. H. McGaughey, "Thermal conductivity of compound semiconductors: Interplay of mass density and acoustic-optical phonon frequency gap." *Journal of Applied Physics* **116**, 073503 (2014).

55. D. Guo, J. Gao, Y.-J. Yu, S. Santhanam, G. K. Fedder, A. J. H. McGaughey, and S. C. Yao, "Electrocaloric characterization of a poly(vinylidene fluoride-trifluoroethylene-chlorofluoroethylene) terpolymer by infrared imaging." *Applied Physics Letters* **105**, 031906 (2014).

54. Q. Zhu, C. Fleck, W. A. Saidi, A. J. H. McGaughey, and J. C. Yang, "TFOx: A versatile kinetic Monte Carlo program for simulations of island growth in three dimensions." *Computational Materials Science* **91**, 292-302 (2014).

53. J. M. Larkin and A. J. H. McGaughey, "Thermal conductivity accumulation in amorphous silica and amorphous silicon." *Physical Review B* **89**, 144303 (2014).

52. W.-L. Ong, S. Majumdar, J. A. Malen, and A. J. H. McGaughey, "Coupling and transport of organic and inorganic vibrational states and their thermal transport in nanocrystal arrays." *Journal of Physical Chemistry C* **118**, 7288-7295 (2014).

51. D. Guo, J. Gao, Y.-J. Yu, S. Santhanam, A. Slippey, G. K. Fedder, A. J. H. McGaughey, and S. C. Yao, "Design and modeling of a fluid-based micro-scale electrocaloric refrigeration system." *International Journal of Heat and Mass Transfer* **72**, 559-564 (2014).

50. P. Li, L. Hu, A. J. H. McGaughey, and S. Shen, "Crystalline polyethylene nanofibers with the theoretical limit of Young's modulus." *Advanced Materials* **26**, 1065-1070 (2014).

49. J. M. Larkin, J. E. Turney, A. D. Massicotte, C. H. Amon, and A. J. H. McGaughey, "Comparison and evaluation of spectral energy methods for predicting phonon properties." *Journal of Computational and Theoretical Nanoscience* **11**, 257-264 (2014).

48. S. C. Huberman, J. M. Larkin, A. J. H. McGaughey, and C. H. Amon, "Disruption of superlattice phonons by interfacial mixing." *Physical Review B* **88**, 155311 (2013).

47. L. Hu and A. J. H. McGaughey, "Energy accommodation between noble gases and carbon nanotubes." *Journal of Physical Chemistry C* **117**, 18804-18808 (2013).

46. D. Guo, J. Gao, A. J. H. McGaughey, G. K. Fedder, M. Moran, and S. C. Yao, "Design and evaluation of a MEMS-based Stirling microcooler." *Journal of Heat Transfer* **135**, 111003 (2013).

45. D. Guo, A. J. H. McGaughey, J. Gao, G. K. Fedder, M. Lee, and S.-C. Yao, "Multiphysics modeling of a micro-scale Stirling refrigeration system." *International Journal of Thermal Sciences* **74**, 44-52 (2013).

44. Y. Wang, B. Qiu, A. J. H. McGaughey, X. Ruan, and X. Xu, "Mode-wise thermal conductivity of bismuth telluride." *Journal of Heat Transfer* **135**, 091102 (2013). **Best Paper, ASME Heat Transfer Division, 2015**.

43. J. M. Larkin and A. J. H. McGaughey, "Predicting alloy vibrational modes properties using lattice dynamics calculations, molecular dynamics simulations, and the virtual crystal approximation." *Journal of Applied Physics* **114**, 023507 (2013).

42. A. Jain, Y.-J. Yu, and A. J. H. McGaughey, "Phonon transport in periodic silicon nanoporous films with feature sizes greater than 100 nm." *Physical Review B* **87**, 195301 (2013).

41. W.-L. Ong, S. M. Rupich, D. V. Talapin, A. J. H. McGaughey, and J. A. Malen, "Surface chemistry mediates thermal transport in three dimensional nanocrystal arrays." *Nature Materials* **12**, 410-415 (2013).

40. K. T. Regner, D. P. Sellan, Z. Su, C. H. Amon, A. J. H. McGaughey, and J. A. Malen, "Broadband phonon mean free paths measured using frequency domain thermoreflectance." *Nature Communications* **4**, 1640 (2013).

39. W. A. Saidi, M. Lee, L. Li, G. Zhou, and A. J. H. McGaughey, "Ab initio atomistic thermodynamics study of the early stages of Cu(100) oxidation." *Physical Review B* **86**, 245429 (2012).

38. S. N. Schiffres, K. H. Kim, L. Hu, A. J. H. McGaughey, M. F. Islam, and J. A. Malen, "Gas diffusion, energy transport, and thermal accommodation in single-walled carbon nanotube aerogels." *Advanced Functional Materials* **22**, 5251-5258 (2012).

37. A. J. H. McGaughey and A. Jain, "Nanostructure thermal conductivity prediction by Monte Carlo sampling of phonon free paths." *Applied Physics Letters* **100** 061911 (2012).

36. D. P. Sellan, E. S. Landry, K. Sasihithlu, A. Narayanaswamy, A. J. H. McGaughey, and C. H. Amon, "Phonon transport across a vacuum gap." *Physical Review B* **85**, 024118 (2012).

35. A. Chernatynskiy, J. E. Turney, A. J. H. McGaughey, C. H. Amon, and S. R. Phillpot, "Phonon-mediated thermal conductivity in ionic solids by lattice-dynamics based methods." *Journal of the American Ceramic Society* **94**, 3523-3531 (2011).

34. A. J. H. McGaughey, E. S. Landry, D. P. Sellan, and C. H. Amon, "Size-dependent model for thin film and nanowire thermal conductivity." *Applied Physics Letters* **99** 131904 (2011).

33. B. Devine, T.-Z. Shan, Y.-T. Cheng, A. J. H. McGaughey, M. Lee, S. R. Phillpot, and S. B. Sinnott, "Atomistic simulations of copper oxidation and Cu/Cu2O interfaces using charge-optimized many-body potentials." *Physical Review B* **84** 125308 (2011).

32. M. Lee and A. J. H. McGaughey, "Energetics and kinetics of the $c(2 \times 2)$ to $(2\sqrt{2} \times \sqrt{2})R45$ transition during the early stages of Cu(100) oxidation." *Physical Review B* **83** 165447 (2011).

31. D. P. Sellan, J. E. Turney, A. J. H. McGaughey, and C. H. Amon, "Cross-plane phonon transport in thin films." *Journal of Applied Physics* **108**, 113524 (2010).

30. D. P. Sellan, E. S. Landry, J. E. Turney, A. J. H. McGaughey, and C. H. Amon, "Size effects in molecular dynamics thermal conductivity predictions." *Physical Review B* **81**, 214305 (2010).

29. M. Lee and A. J. H. McGaughey, "Role of sub-surface oxygen in Cu(100) oxidation." *Surface Science* **604**, 4125-1431 (2010).

28. J. A. Thomas, J. E. Turney, R. M. Iutzi, C. H. Amon and A. J. H. McGaughey, "Predicting phonon dispersion relations and lifetimes from the spectral energy density." *Physical Review B* **81**, 081411(R) (2010).

27. J. E. Turney, A. J. H. McGaughey, and C. H. Amon, "In-plane phonon transport in thin films." *Journal of Applied Physics* **107**, 024317 (2010).

26. E. S. Landry and A. J. H. McGaughey, "Effect of film thickness on the thermal resistance of confined semiconductor thin films." *Journal of Applied Physics* **107**, 013521 (2010).

25. J. A. Thomas, R. M. Iutzi, and A. J. H. McGaughey, "Thermal conductivity and phonon transport in empty and water-filled carbon nanotubes." *Physical Review B* **81**, 045413 (2010).

24. J. A. Thomas, A. J. H. McGaughey, and O. Kuter-Arneback, "Pressure-driven water flow through carbon nanotubes: Insights from molecular dynamics simulations." *International Journal of Thermal Sciences* **49**, 481-489 (2010).

23. M. Lee and A. J. H. McGaughey, "Energetics of oxygen embedment into unreconstructed and reconstructed Cu(100) surfaces: Density functional theory calculations." *Surface Science* **603**, 3404-3409 (2009).

22. E. S. Landry and A. J. H. McGaughey, "Thermal boundary resistance predictions from molecular dynamics simulations and theoretical calculations." *Physical Review B* **80** 165304 (2009).

21. J. E. Turney, A. J. H. McGaughey, and C. H. Amon, "Assessing the applicability of quantum corrections to classical thermal conductivity predictions." *Physical Review B* **79**, 224305 (2009).

20. J. A. Thomas and A. J. H. McGaughey, "Water flow in carbon nanotubes: Transition to subcontinuum flow." *Physical Review Letters* **102**, 184502 (2009).

19. E. S. Landry and A. J. H. McGaughey, "Effect of interfacial species mixing on phonon transport in semiconductor superlattices." *Physical Review B* **79**, 075316 (2009).

18. J. E. Turney, E. S. Landry, A. J. H. McGaughey, and C. H. Amon, "Predicting phonon properties and thermal conductivity from anharmonic lattice dynamics calculations and molecular dynamics simulations." *Physical Review B* **79**, 064301 (2009).

17. S. Shenogin, A. Bodapati, P. Keblinski, and A. J. H. McGaughey, "Predicting the thermal conductivity of inorganic and polymeric glasses: The role of anharmonicity." *Journal of Applied Physics* **105**, 034906 (2009).

16. S. E. Jee, A J. H. McGaughey, and D. S. Sholl, "Molecular simulations of hydrogen and methane permeation through pore mouth modified zeolite membranes." *Molecular Simulation* **35**, 70-78 (2009).

15. J. A. Thomas and A. J. H. McGaughey, "Reassessing fast water transport through carbon nanotubes," *Nano Letters* **8**, 2788-2793 (2008).

14. E. S. Landry, M. I. Hussein, and A. J. H. McGaughey, "Complex superlattice unit cell designs for reduced thermal conductivity." *Physical Review B* **77**, 184302 (2008).

13. J. A. Thomas and A. J. H. McGaughey, "Density, distribution, and orientation of water molecules inside and outside carbon nanotubes." *Journal of Chemical Physics* **128**, 084715-1-6 (2008).

12. E. S. Landry, S. Mikkilineni, M. Paharia, and A. J. H. McGaughey, "Droplet evaporation: A molecular dynamics investigation." *Journal of Applied Physics* **102**, 124301-1-7 (2007).

11. J. A. Thomas and A. J. H. McGaughey, "Effect of surface wettability on liquid density, structure, and diffusion near a solid surface." *Journal of Chemical Physics* **126**, 034707 (2007).

10. B. L. Huang, A. J. H. McGaughey, and M. Kaviany, "Thermal conductivity of metal-organic framework 5 (MOF-5): Part I. Molecular dynamics simulations." *International Journal of Heat and Mass Transfer* **50**, 393-404 (2007).

9. B. L. Huang, Z. Ni, A. Millward, A. J. H. McGaughey, C. Uher, M. Kaviany, and O. Yaghi "Thermal conductivity of metal-organic framework 5 (MOF-5): Part II. Measurement." *International Journal of Heat and Mass Transfer* **50**, 405-411 (2007).

8. A. J. H. McGaughey, M. I. Hussein, E. S. Landry, M. Kaviany, and G. Hulbert, "Phonon band structure and thermal transport correlation in a layered diatomic crystal." *Physical Review B* **74**, 104304 (2006).

7. A. J. H. McGaughey and M. Kaviany, "Observation and description of phonon interactions in molecular dynamics simulations." *Physical Review B* **71**, 184305 (2005).

6. J. D. Chung, A. J. H. McGaughey, and M. Kaviany, "Role of phonon dispersion in lattice thermal conductivity analysis." *Journal of Heat Transfer* **126**, 376-380 (2004).

5. A. J. H. McGaughey and M. Kaviany, "Quantitative validation of the Boltzmann transport equation phonon thermal conductivity model under the single-mode relaxation time approximation." *Physical Review B* **69**, 094303 (2004).

4. A. J. H. McGaughey and M. Kaviany, "Thermal conductivity decomposition and analysis using molecular dynamics simulations. Part I. Lennard-Jones argon." *International Journal of Heat and Mass Transfer* **47**, 1783-1798 (2004).

3. A. J. H. McGaughey and M. Kaviany, "Thermal conductivity decomposition and analysis using molecular dynamics simulations. Part II. Complex silica crystals." *International Journal of Heat and Mass Transfer* **47**, 1799-1816 (2004).

2. A. J. H. McGaughey and C. A. Ward, "Stability of a droplet in a finite system: Consideration of the solid-vapor interface." *Journal of Applied Physics* **93**, 3619-3626 (2003).

1. A. J. H. McGaughey and C. A. Ward, "Temperature discontinuity at the surface of an evaporating droplet." *Journal of Applied Physics* **91**, 6406-6415 (2002).

Other Writings

5. A. J. H. McGaughey and D. Mattia, "Materials enabling nanofluidic flow enhancement." *MRS Bulletin*, April 2017, 273-275.

4. A. J. H. McGaughey, "Relaxons heat up thermal transport." Viewpoint in *Physics*, **9** 118 (October 17, 2016).

3. B. A. Cola, H. Daiguji, C. Dames, N. Fang, K. Fushinobu, S. Inoue, G. Kikugawa, M. Kohno, S. Kumar, D. Y. Li, J. R. Lukes, J. A. Malen, A. J. H. McGaughey, O. Nakabeppu, K. Pipe, P. Reddy, S. Shen, L. Shi, M. Shibahara, Y. Taguchi, K. Takahashi, T. Yamamoto, and T. Zolotoukhina, "Report on the Seventh U.S.-Japan Joint Seminar on Nanoscale Transport Phenomena-Science and Engineering," *Nanoscale and Microscale Thermophysical Engineering* **17** 25-49 (2013).

2. A. J. H. McGaughey, "Modeling thermoelectric materials and devices." *American Ceramic Society Bulletin* **91**, Volume 3, 34-38 (2012).

1. S. R. Phillpot and A. J. H. McGaughey, "Introduction to thermal transport," *Materials Today*, 18-20, June 2005.

Invited Seminars

45. "Integrating theory, simulation, machine learning, and experiments to solve heat transfer problems." Stevens Institute of Technology, Department of Mechanical Engineering, November 2022.

44. "Integrating theory, simulation, machine learning, and experiments to solve heat transfer problems." Viskanta Lecture, Purdue University, Department of Mechanical Engineering, November 2021.

43. "Thermal transport in large unit cell crystals." University of Virginia, Department of Mechanical and Aerospace Engineering, October 2020 (virtual).

42. "Phonon transport and confinement in thin films." Dalhousie University, Department of Physics & Atmospheric Science, Halifax, Nova Scotia, Canada, October 2019.

41. "Thermal transport in large unit cell crystals." Massachusetts Institute of Technology, S^3TEC, February 2018.

40. "Atomistic modeling of thermal transport." University of Pittsburgh, Department of Mechanical Engineering and Materials Science, November 2017.

39. "Atomistic modeling of thermal transport." University of California, Los Angeles, Department of Mechanical Engineering, October 2017.

38. "Next generation materials for energy transport and conversion: Growth, characterization, and modeling." Northrop Grumman Next, Redondo Beach, CA, October 2017 (with Jonathan Malen and Xavier Roy).

37. "Atomistic modeling of thermal transport." Carnegie Mellon University, Department of Materials Science and Engineering, September 2017.

36. "Thermal transport by phonons and electrons from first principles calculations," University of Tokyo, Department of Mechanical Engineering, June 2017.

35. "Thermal transport in organic-inorganic heterostructures," University of Tokyo, Institute of Industrial Science, June 2017.

34. "Thermal transport in organic-inorganic heterostructures," Pontificia Universidad Catolica de Chile, Department of Mechanical Engineering, Santiago, Chile, January 2017.

33. "Thermal transport in organic-inorganic heterostructures," University of California, San Diego, Department of Mechanical Engineering November 2016.

32. "Thermal transport by phonons and electrons from first principles calculations," Cornell University, Department of Materials Science and Engineering, September 2016.

31. "Thermal transport by phonons and electrons from first principles calculations," University of Colorado, Boulder, Department of Aerospace Engineering Sciences, June 2016.

30. "Thermal transport by phonons and electrons from first principles calculations," Sandia National Laboratory, Albuquerque, NM, June 2016.

29. "Phonon properties and thermal conductivity of 3-D and 2-D crystals," Ecole Polytechnique, Paris, France, March 2016.

28. "Thermal transport across organic-inorganic interfaces," Ohio State University, Department of Mechanical and Aerospace Engineering, October 2015.

27. "Nanoscale thermal transport: Formulation for modeling at the atomic scale," "Phonon properties and thermal conductivity of 3-D and 2-D crystals," "Vibrational mode properties and thermal conductivity of disordered solids," and "Thermal transport across organic-inorganic interfaces," Xi'an Jiaotong University, Xi'an, China, September 2015.

26. "Thermal transport across organic-inorganic interfaces," Universite Lyon I, Lyon, France, July 2015.

25. "Thermal transport across organic-inorganic interfaces," Universite de Lorraine, Nancy, France, June 2015.

24. "Phonon properties and thermal conductivity from atomistic calculations," and "Thermal transport across organic-inorganic interfaces," Centrale Superlec, Paris, France, June 2015.

23. "Phonon Properties and Thermal Conductivity from Atomistic Calculations," University of Michigan, Department of Mechanical Engineering, May 2015.

22. "Thermal transport across organic-inorganic interfaces," University of Toronto, Departments of Mechanical and Electrical & Computer Engineering, April 2015.

21. "Thermal transport across organic-inorganic interfaces," University of Alberta, Department of Chemical and Materials Engineering, July 2014.

20. "Phonon properties and thermal conductivity from atomistic calculations," University of California, Berkeley, Department of Mechanical Engineering, July 2014.

19. "Predicting thermal conductivity from molecular dynamics simulations" and "Predicting phonon properties from molecular dynamics simulations," lectures at 2nd International Conference on Phononics and Thermal Energy Science, Shanghai, China, May 2014.

18. "Measuring and predicting thermal transport properties," tutorial at the 2013 MRS Spring Meeting (with A. Shakouri), San Francisco, CA, April 2013.

17. "Quantum mechanics-driven prediction of nanostructure thermal Conductivity," University of Houston, Department of Mechanical Engineering, February 2013.

16. "Transport phenomena in nanostructures," Carnegie Mellon University, Department of Mechanical Engineering, February 2013.

15. "Quantum mechanics-driven prediction of nanostructure thermal Conductivity," University of North Texas, Department of Mechanical and Energy Engineering, January 2013.

14. "Quantum mechanics-driven prediction of nanostructure thermal conductivity," University of Texas Austin, Department of Mechanical Engineering, September 2012.

13. "Quantum mechanics-driven prediction of nanostructure thermal conductivity," Air Force Research Laboratory, Dayton, OH, June 2012.

12. "Thermal transport by phonons in thin films," University of Tokyo, Department of Mechanical Engineering, December 2011.

11. "Thermal transport by phonons in thin films," Rensselaer Polytechnic Institute, Department of Materials Science and Engineering, November 2011.

10. "Thermal transport by phonons in thin films," Vanderbilt University, Department of Mechanical Engineering, October 2011.

9. "Thermal transport by phonons in thin films," Korea Advanced Institute of Science and Technology, Department of Mechanical Engineering, July 2011.

8. "Fluid flow and heat transfer in carbon nanotubes," Columbia University, Department of Mechanical Engineering, October 2009.

7. "Phonon transport in semiconductor superlattices," Georgia Tech, Structural Materials Seminar Series, September 2009.

6. "Nanoscale transport phenomena: Insights from molecular simulation," Carnegie Mellon University, Department of Mechanical Engineering, May 2009.

5. "Water structure and flow inside carbon nanotubes," University of Pittsburgh, January 2009.

4. "Molecular dynamics simulations: Introduction and application to transport problems," Carnegie Mellon University, Process Systems Engineering Seminar, November 2005.

3. "Atomic structure and phonon thermal conductivity: Molecular dynamics investigation in real and phonon spaces," University of Minnesota, Department of Mechanical Engineering, June 2004.

2. "Atomic structure and phonon thermal conductivity: Molecular dynamics investigation in real and phonon spaces," Carnegie Mellon University, Department of Mechanical Engineering, April 2004.

1. "Atomic structure and phonon thermal conductivity: Molecular dynamics investigation in real and phonon spaces," Los Alamos National Laboratory, March 2004.

Conference and Workshop Activities (speaker in bold)

Full list of contributed presentations at end of CV.

Invited

28. (Keynote) **A. J. H. McGaughey**,"Integrating theory, simulation, machine learning, and experiments to solve heat transfer problems." Oak Ridge Postdoctoral Association Research Symposium, July 2022 (virtual).

27. **A. J. H. McGaughey**, "Ultrahigh evaporative heat transfer measured locally in submicron water films interpreted by a data-driven analysis." international Center for Theoretical Physics meeting on Recent Progress in Thermal Transport Theory and Experiments, June 2022 (virtual).

26. **A. J. H. McGaughey**, H. T. Aller, and J. A. Malen, "Universal model for predicting the thermal boundary conductance of a multilayered-metal/dielectric interface." MRS 2021 Fall Meeting (virtual).

25. **A. J. H. McGaughey**, H. T. Aller, and J. A. Malen, "Universal model for predicting the thermal boundary conductance of a multilayered-metal/dielectric interface." XXIX International Materials Research Congress, August 2021 (virtual).

24. **A. J. H. McGaughey**, Q. Liang, W.-L. Ong, M. Bartnof, Y.-L. He, X. Roy, and J. A. Malen, "Thermal transport and fullerene dynamics in superatomic crystals." MRS 2021 Spring Meeting (virtual).

23. **A. J. H. McGaughey**, H. L. Parks, H.-Y. Kim, and V. Viswanathan, "Quantifying uncertainty in first-principles predictions of molecular vibrational frequencies, phonon properties, and thermal conductivity." APS March Meeting 2021 (virtual).

22. H.-Y. Kim, B. Fu, K. D. Parrish, and **A. J. H. McGaughey**, "Phonon confinement in thin films." Nanoscale Thermal Transport and Heat Localization, Vancouver, BC, August 2018.

21. **A. J. H. McGaughey**, "Next-Generation Atomistic Modeling of Thermal Transport." ITherm 2018, San Diego, CA, May 2018.

20. **A. J. H. McGaughey**, "Phonon transport modeling." IEEE NANO 2017, Pittsburgh, PA, July 2017.

19. S. Kumar, C. Shao, S. Lu, and **A. J. H. McGaughey**, "Degree-of-freedom resolved thermal transport in the C_{60} molecular crystal," 9th US-Japan Joint Seminar on Nanoscale Transport Phenomena, Tokyo, Japan, July 2017.

18. **A. J. H. McGaughey** and **X. Ruan**, "Phonon transport modeling: Formulation, implementation, and applications." Six tutorials given over two sessions. ASME 2016 IMECE, Phoenix, AZ, November 2016.

17. (Keynote) **A. J. H. McGaughey** and A. Jain, "Thermal transport by phonons and electrons from first principles." Fourth International Conference on Computational Methods for Thermal Problems (ThermaComp2016), Atlanta, GA, July 2016.

16. **A. J. H. McGaughey**, "Vibrational mode properties in disordered solids." CECAM worksop on "Advanced thermoelectrics at nanoscale: From materials to devices," Paris, France, July 2015.

15. **A. J. H. McGaughey**, "Vibrational mode properties in disordered solids." 6th International Symposium on Advances in Computational Heat Transfer, Piscataway, NJ, May 2015.

14. **A. J. H. McGaughey**, W. L. Ong, S. Majumdar, and J. A. Malen, "Thermal transport across organic-inorganic interfaces," 8th US-Japan Joint Seminar on Nanoscale Transport Phenomena, Santa Cruz, CA, July 2014.

13. **A. J. H. McGaughey** and A. Jain "Phonon transport in periodic silicon nano porous films," 2nd International Conference on Phononics and Thermal Energy Science, Shanghai, China, May 2014.

12. **A. J. H. McGaughey**, A. Jain, J. M. Larkin, E. S. Landry, S. C. Huberman, C. H. Amon, "Phonon transport in periodic materials with feature sizes of 1 nm to 1 mm." AMERIMECH Symposium on Dynamics of Periodic Materials and Structures, Atlanta, GA, April 2014.

11. **A. J. H. McGaughey**, W. L. Ong, S. Majumdar, and J. A. Malen, "Atomic modeling of thermal transport in hybrid organic-inorganic materials." MRS 2013 Spring Meeting, San Francisco, CA, April 2013.

10. **A. J. H. McGaughey**, W. L. Ong, S. Majumdar, and J. A. Malen, "Atomistic modeling of thermal transport in nanocrystal superlattices and self-assembled monolayer junctions." ASME 2012 IMECE, Houston, TX, November 2012.

9. **A. J. H. McGaughey**, "Combining atomistic calculations and the Boltzmann transport equation to predict nanostructure thermal conductivity." Averaging Methods for Multiscale Phenomena in Engineering Materials Workshop, Pittsburgh PA, April 2012.

8. **A. J. H. McGaughey**, A. Jain, J. E. Turney, D. P. Sellan, and C. H. Amon, "Thermal transport in thin films," 7th US-Japan Joint Seminar on Nanoscale Transport Phenomena, Shima, Japan, December 2011.

7. **A. J. H. McGaughey**, J. E. Turney, J. A. Thomas, H. Chen, R. M. Iutzi, A. D. Massicotte, and C. H. Amon, "Predicting phonon properties using the spectral energy density." Phononics 2011, Santa Fe, NM, May 2011.

6. **A. J. H. McGaughey**, "Predicting phonon properties using lattice dynamics calculations and molecular dynamics simulation." Third International Workshop on Transmission of Information and Energy in Nonlinear and Complex Systems, Singapore, July 2010.

5. **A. J. H. McGaughey** and E. S. Landry, "Thermal transport across semiconductor interfaces and thin films." Spring 2010 MRS Meeting, April 2010, San Francisco, CA.

4. J. A. Thomas, R. M. Iutzi, J. E. Turney, and **A. J. H. McGaughey**, "Coupling between phonons and fluid particles in water/carbon nanotube systems," ASME paper MNHMT2009-18305, ASME 2009 Micro/Nanoscale Heat and Mass Transfer International Conference, Shanghai, China, December 2009.

3. **J. A. Thomas** and A. J. H. McGaughey, "Water transport through carbon nanotubes: Insights from molecular dynamics simulation." Nanobiophysics, Nanochemistry, Nanomedicine & Nanotoxicology Conference 2009, January 2009, Antigua.

2. **A. J. H. McGaughey** and E. S. Landry, "Exploration of superlattice thermal conductivity tensor design space," Spring 2007 MRS Meeting, San Francisco CA, April 2007.

1. **A. J. H. McGaughey**, "Analysis of phonon transport in superlattices using molecular dynamics simulations." CECAM workshop on "Heat transfer simulation at the atomic scale: New challenges for the future," Lyon, France, September 2006.

Research Funding

As PI

- "Thermal Performance of Ultra-Wide Bandgap Materials and Devices Under Extreme Fields." $150,000 (to date). Army Research Office. September 2022-. Co-PIs: J. A. Malen (CMU), S. Choi (Penn State University).
- "Vibrational structure and thermal transport in statically and dynamically disordered crystals." $360,000. National Science Foundation, January 2021 - December 2023.
- "Thermally-stable halide perovskites for photovoltaic energy conversion." $75,000, Wilton E. Scott Institute for Energy Innovation, March 2019-June 2020. Co-PI: J. A. Malen (CMU).
- "Electrocaloric cooling in polymers: Multi-scale modeling and experimental characterization." $360,000. National Science Foundation, August 2016 - July 2019. Co-PI: S. C. Yao (CMU).
- "Thermal transport in large unit cell crystals." $330,000. National Science Foundation, July 2015 - June 2018.
- "Heat transfer enhancement in nanoscale film evaporation." $57,000, Pennsylvania Infrastructure Technology Alliance. January 2014 - May 2015. Other PI: J. A. Malen (CMU), co-PI S. C. Yao (CMU).
- "Phonon transport near and across semiconductor interfaces." $300,000. National Science Foundation, September 2010 - August 2013. Co-PI: Y. Wang (Pittsburgh Supercomputing Center)
- "Quantum mechanics-driven prediction of nanostructure thermal conductivity." $361,640. Air Force Office of Scientific Research (Young Investigator Program), May 2010 - April 2013.
- "IDR: Carbon nanotube aerogels for next-generation thermal management." $965,874. National Science Foundation, September 2009 - August 2012. Co-PIs S. Anna and M. Islam (CMU) and K. Pipe (Michigan).
- "Multiscale modeling of phase change materials." $44,175, Pennsylvania Infrastructure Technology Alliance. January 2009 - May 2010. Co-PI J. Bain (CMU).
- "Atomistic characterization and modeling of deep sub-micron gate oxide breakdown." $64,410. Pennsylvania Infrastructure Technology Alliance. January 2008 - May 2009. Co-PI R. F. Davis (CMU).
- "Kapitza conductance of solid-solid interfaces," $8,790. Berkman Faculty Development Fund, Carnegie Mellon University. January 2006-December 2006.

As co-PI

- "Electric field- and light-modulated thermal transport in superatomic crystals." $289,999 (CMU portion). NSF. August 2020-July 2023. PI: J. A. Malen (CMU). Other co-PI: Xavier Roy (Columbia).
- "AI driven investigation of the physics of field-matter coupling for materials synthesis." $995,723. DARPA. December 2018-May 2020. PI: A. Singh. Other co-PIs: A. Davis, B. R. Jayan.
- "Physical behavior of layered superatomic crystals." $626,372. Army Research Office. October 2017-September 2010. PI: J. A. Malen (CMU). Other co-PI: Xavier Roy (Columbia).
- "Metal alloys for thermal engineering of advanced electronics." $385,000. Northrup Grumman. August 2016-December 2020. PI: J. A. Malen (CMU). Other co-PI: A. Gellman (CMU).
- "Phosphor conversion matrix with high thermal conductivity for next-generation phosphor-converted LED-based solid state lighting." $1,934,774. Department of Energy. August 2014 - November 2016. PI: M. Bockstaller, nine other co-Pis.
- "GOALI: Thermal transport by phonons in device-grade nitride nanostructures." $430,284. National Science Foundation. September 2011-August 2014. PI: J. A. Malen (CMU). Other co-PI: R. F. Davis (CMU).
- "Stirling microcooler array with elemental in-plane flow." $2,600,000. DARPA, June 2010 - May 2013. PI: G. Fedder (CMU). Other co-PIs: W. Anderson (Active Cooling Technologies), M. Moran (Isotherm), and S. C. Yao (CMU).
- "Multiscale atomistic simulation of metal-oxygen surface interactions: methodological development, theoretical investigation and correlation with experiment." $641,301. Department of Energy, Basic Energy Sciences. October 2007-August 2010. PI: J. Yang (Pittsburgh). Other co-PIs: S. R. Phillpot and S. B. Sinnott (Florida).
- "Multiscale atomistic simulation of metal-oxygen surface interactions: methodological development, theoretical investigation and correlation with experiment." $148,000. Department of Energy, Basic Energy Sciences. January 2006-June 2007. PI: J. Yang (Pittsburgh). Other co-PIs: S. R. Phillpot and S. B. Sinnott (Florida).

Contributions to Education

Teaching at Carnegie Mellon University

Course	Units	Offered	Students/ Response	FCE Course	FCE Instructor
24-739: Molecular Simulation of Materials	12	S06	15/13	4.7	4.8
24-703: Numerical Methods in Mech. Eng.	12	F06	39/30	3.9	4.1
24-739: Molecular Simulation of Materials	12	S07	14/8	4.0	4.3
24-734: Small Scale Heat Transfer	6	S07	7/7	3.9	4.3
24-703: Numerical Methods in Mech. Eng.	12	F07	41/29	4.45	4.72
24-701: Math. Techniques in Mech. Eng.	12	S08	25/20	4.25	4.63
24-322: Heat Transfer	10	F08	101/67	4.26	4.46
24-703: Numerical Methods in Mech. Eng.	12	S09	31/31	4.61	4.84
24-322: Heat Transfer	10	F09	97/80	4.16	4.36
24-623: Molecular Simulation of Materials	12	S10	22/19	4.89	4.89
24-322: Heat Transfer	10	F10	99/82	4.51	4.63
24-623: Molecular Simulation of Materials	12	S11	17/15	4.94	5.00
24-322: Heat Transfer	10	F11	89/67	4.61	4.81
24-623: Molecular Simulation of Materials	12	S12	18/17	4.82	4.89
24-311: Numerical Methods	12	F13	123/99	4.30	4.44
24-101: Fundamentals of Mechanical Eng.	12	S14	129/76	3.72	3.97
24-311: Numerical Methods	12	F14	108/72	4.37	4.51
24-101: Fundamentals of Mechanical Eng.	12	S15	115/57	3.72	4.11
24-623: Molecular Simulation of Materials	12	F15	19/16	4.94	4.94
24-311: Numerical Methods	12	S16	128/85	4.60	4.69
24-623: Molecular Simulation of Materials	12	F16	16/10	4.90	4.90
24-231: Fluid Mechanics	10	S17	172/113	4.29	4.42
24-623: Molecular Simulation of Materials	12	F17	29/23	4.83	5.00
24-231: Fluid Mechanics	10	S18	118/72	4.49	4.61
24-623: Molecular Simulation of Materials	12	F18	32/25	4.92	5.00
24-231: Fluid Mechanics	10	S19	125/71	4.46	4.58
24-703: Numerical Methods in Engineering	12	F19	48/37	4.89	4.97
24-623: Molecular Simulation of Materials	12	S20	20/17	4.83	4.94
24-311: Numerical Methods (R)	12	F20	22/15	4.87	5.00
24-703: Numerical Methods in Engineering (R)	12	F21	43/42	4.64	4.79
24-322: Heat Transfer	10	F22	119/71	4.34	4.48
24-703: Numerical Methods in Engineering	12	S23	36/20	4.35	4.30

Mechanical Engineering Department historical averages: Course: 4.0, Instructor: 4.1.
R = remote teaching

Innovation

- Developed the new course 24-623: Molecular Simulation of Materials and taught it ten times. Made a series of videos.
- Created active learning modules for 24-311: Numerical Methods, 24-703: Numerical Methods in Mechanical Engineering, and 23-623: Molecular Simulation of Materials. This work formed the basis for my contribution to the 2015 National Academy of Engineering Frontiers of Engineering Education Symposium.
- As the Struminger Junior Faculty Fellow in 2009, I designed two new laboratory demonstrations for 24-322: Heat Transfer.
- Developed the lecture series "Mechanical Engineering from the Nanometer-Up."

Publications

- A. J. H. McGaughey and J. J. Michalek, "Wiki-based learning in the mechanical engineering classroom," 2008 ASEE Annual Conference and Exposition, June 2008, Pittsburgh, PA.
- E. R. Chan, S. P. Holleran, A. J. H. McGaughey, and C. Rasmussen, "ASEE student chapters: Avenues for promoting future engineering educators," 2004 ASEE Annual Conference and Exposition, June 2004, Salt Lake City, UT.

Previous Experience

- University of Michigan, January-April 2001, September-December 2001. Course: ME330: Thermal & Fluid Sciences II, Graduate Student Instructor (GSI).
- University of Toronto, September 1998-April 2000. Courses: MIE 310: Thermodynamics, MIE 313: Heat Transfer and MIE 100: Dynamics, Teaching Assistant (TA).
- Vice-President, University of Michigan ASEE Graduate Student Chapter, May 2003-May 2004.

Service at Carnegie Mellon University

Mechanical Engineering Department

- Seminar Committee (2006-2008)
- Computer Committee (2006-2010)
- Organizer of qualifier exams: Fall 2010, Spring 2011, Fall 2011, Spring 2012
- Mechanical Engineering Graduate Student Organization advisor (2008-2010)
- Graduate Student Research Conference coordinator (2010, 2011)
- Awards Committee (Chair, 2013-2016)
- Graduate Education Committee (2008-2012, 2015-2020),
  Chair (2016-2020). Major responsibilities and accomplishments as Chair:
  - Manage committee of twelve faculty and two staff
  - Oversee PhD and Masters admissions and programs (400+ students)
  - Led graduate education portion of department external review (2018) and strategic plan (2019-20)
  - Design, approval, and rollout of a new Masters program
  - Institution of a new award for best PhD Dissertation
  - Implementation of a new PhD student annual review process
  - Standardization of policy-related processes (e.g., petitions, degree progress)
  - Adding educational components to Teaching Assistant experience
- Undergraduate Education Committee (2021)
- Faculty Search Committee (Chair) (2022-)

College of Engineering

- Civil & Environmental Engineering faculty search (2006)
- Curriculum Review Committee (2010-2012)
- Strategic Planning Committee (2013)
- Center for Faculty Success, Junior Faculty Lead (2015-2020) Major accomplishments:
  - Design and organization of a new orientation for new faculty members
  - Organize and run sessions for junior faculty applying for early career awards
  - Interviewed faculty and reported back to Dean about mentoring and feedback
  - Run "Bias Busters" sessions to remove unconscious bias and increase diversity
- Dean Evaluation Committee (2018)
- Faculty Chair Elect (2018) and Faculty Chair (2019-2020). Responsibilities:
  - Member of College Awards Committee
  - Attend College Council meetings, where Department Heads present proposed curriculum changes
  - Attend Review of Promotion and Tenure meetings, where Department Heads present cases to the Dean
- Dean Search Advisory Committee (2019)

University

- University Committee on Faculty Appointments Without Indefinite Tenure (2011-2012)
- Physics faculty search (2011-2012)
- Goldwater Award selection committee (2014-2017)
- Berkman Faculty Development Fund selection committee (2016-2018)
- DSF Charitable Foundation selection committee (2017)
- University Committee on Appointments with Indefinite Tenure (2021-2023)

Professional Activities

ASME

- Member (2003-), Fellow (2016)
- *Journal of Heat Transfer* Associate Editor (2015-2018)
  - Special recognition for "Exceptional Service"
- *Journal of Heat Transfer*, Outstanding Reviewer (2011)
- Member, ASME Heat Transfer Division K-8 (Theory and Fundamental Research) Committee (2006-).
- Track organizer, 2013 ASME Summer Heat Transfer Conference.
- Track organizer, 2018 IMECE.
- Session organizer and chair, 2008, 2009, and 2012 ASME Summer Heat Transfer Conferences, 2011 ASME/JSME Thermal Engineering Joint Conference, 2013 IMECE.

APS

- Member (2005-)
- Fellow, Division of Materials Physics (2021). Citation: For significant contributions to the development and advancement of theoretical and computational methods for the determination and fundamental understanding of thermal conductivity.
- Organizing committee, 2013 APS Division of Fluid Dynamics Meeting.
- Outstanding Reviewer, 2015.
- *Physical Review B* ad hoc Editorial Board member, 2021.

MRS

- Member (2007-)
- Symposium organizer, 2011 MRS Spring Meeting. Co-organizers: Ming Su (U. Central Florida), Shawn Putnam (Air Force), Junichiro Shiomi (U. Tokyo).
- *MRS Bulletin* Guest Editor (with Davide Mattia), April 2017 issue on "Materials enabling nanofluidic flow enhancement."

Other Conference and Workshop Organization

- Co-organizer (with D. Leitner), Telluride Science Research Center June 2010 and June 2013 workshops "Thermal transport at the nanoscale," Telluride, CO.
- Organizer, May 2013 Harrington Symposium, "Next-generation materials for energy generation, storage, and transport," Austin, TX.
- Co-organizer (with D. Donadio), CECAM workshop "Advanced thermoelectrics at nanoscale: from materials to devices." Lugano, Switzerland, June 2011.
- Symposium organizer, "Characterization and modeling of ceramic-ceramic and metal-ceramic interfaces," Materials Science & Technology Conference, 2009. Co-organizers: Judith Yang (U. Pittsburgh), Susan Sinnott (U. Florida).
- Organizer of "Simulators' Meeting," Carnegie Mellon University, 2007-2011 & 2013-2018.

Other

- Reviewer for *ACS Nano, Annual Review of Heat Transfer, Applied Physics Letters, Communications in Nonlinear Science and Numerical Simulation, European Physics Letters, International Journal for Computational Methods in Engineering Science and Mechanics, International Journal of Heat and Fluid Flow, International Journal of Heat and Mass Transfer, Journal of Applied Physics, Journal of Chemical Physics, Journal of Heat Transfer, Journal of Physical Chemistry, Journal of Physical Chemistry Letters, Journal of Physics: Condensed Matter, Langmuir, Microfluidics and Nanofluidics, Nano Letters, Nanoscale, Nanoscale and Microscale Thermophysical Engineering, Nature, Nature Materials, Nature Nanotechnology, Nature Communications, New Journal of Physics, Physics of Fluids, Physical Review Applied, Physical Review B, Physical Review E, Physical Review Letters, Proceedings of the Royal Society A, Reviews of Modern Physics, Scientific Reports*, Department of Energy Office of Basic Energy Sciences, National Science Foundation, Army Research Lab, Office of Naval Research, Petroleum Research Fund.
- Panelist, graduate student workshop on obtaining an academic position, University of Michigan, November 2005, May 2015.

- Speaker for SWE High School Outreach, CMU, 2005-2009.
- YWCA TechGyrls coach, Fall 2008, Spring 2010, Spring 2011, Spring 2012.
- Osher Lifelong Learning Institute at CMU. Five-session short course in 2009. One lecture in 2016.
- Mattress Factory camp "Cartoons and Creations." Volunteer, Summer 2016

Contributed Conference and Workshop Presentations

192. **J. Gong**, S. Chu, R. Mehta, and A. J. H. McGaughey, "Physics-informed XGBoost model for electrocaloric temperature change predictions in ceramics." MRS 2022 Spring Meeting (virtual).

191. **S. Zhang**; J. Gong, B. R. Jayan, and A. J. H. McGaughey, "Data-driven approaches for defect concentration prediction of microwave-synthesized TiO_2. MRS 2022 Spring Meeting (virtual).

190. **S. Zhang**; J. Gong, B. R. Jayan, and A. J. H. McGaughey, "Data-driven approaches on pair distribution function data: matrix factorization and clustering." IUCr 2021, August 2021 (virtual).

189. **H.-Y. Kim** and A. J. H. McGaughey, "Predicting phonon properties and thermal conductivity of crystals with rigid molecules using rotational lattice dynamics." MRS 2021 Spring Meeting (virtual).

188. **H. Parks**, H.-Y. Kim, V. Viswanathan, and A. J. H. McGaughey, "Uncertainty quantification in first-principles predictions of phonon properties and lattice thermal conductivity." MRS 2021 Spring Meeting (virtual).

187. **X. Wang**, S. A. Ghaffarizadeh, A. J. H. McGaughey, and J. A. Malen, "Local study of the evaporation mass flux in a thin liquid film using thermoreflectance experiments and numerical methods." MRS 2021 Spring Meeting (virtual).

186. **X. Wang**, J. Chen, J. A. Malen, and A. J. H. McGaughey, "Anchor-shaped surfactants enhance evaporation on a flat liquid-vapor interface." MRS 2021 Spring Meeting (virtual).

185. **J. A. Malen**, H. Aller, N. Golio, K. Hobart, T. Feygelson, A. J. H. McGaughey, A. Gellman, "Optimizing top-side device cooling via metal/nanocrystalline diamond interfaces." MRS 2021 Spring Meeting (virtual).

184. J. Gong, **H.-Y. Kim**, and A. J. H. McGaughey, "Neural network potential for lattice dynamics calculations and thermal conductivity prediction." APS March Meeting 2021 (virtual).

183. **J. Gong**, R. Mehta, and A. J. H. McGaughey, "Physics-informed data-driven approach for optimizing electrocaloric cooling." APS March Meeting 2021 (virtual).

182. **S. Zhang**, S. Jha, J. Gong, N. Nakamura, A. J. H. McGaughey, and B. R. Jayan,"Structures of point defects in ceramic oxides during microwave radiation-assisted synthesis." MRS 2020 Fall Meeting, December 2020 (virtual).

181. **H. L. Parks**, H.-Y. Kim, V. Viswanathan, and A. J. H. McGaughey, "Quantifying uncertainty in first-principles predictions of phonon properties and lattice thermal conductivity." ASME 2020 IMECE, November 2020 (virtual).

180. **J. Gong**, R. Mehta, and A. J. H. McGaughey, "Physics-informed data-driven approach for optimizing electrocaloric cooling." ASME 2020 IMECE, November 2020 (virtual).

179. **X. Wang**, S. A. Ghaffarizadeh, A. J. H. McGaughey, and J. A. Malen, "Local study of the evaporation mass flux in thin liquid films using experiments and numerical methods." ASME 2020 IMECE, November 2020 (virtual).

178. **X. Wang**, J. Chen, J. A. Malen, and A. J. H. McGaughey, "Anchor-shaped surfactants enhance evaporation on a flat liquid interface." ASME 2020 IMECE, November 2020 (virtual).

177. **H. T. Aller**, N. Golio, K. Hobart, T. Feygelson, A. J. H. McGaughey, A. Gellman, and J. A. Malen, "Optimizing top-side device cooling via metal/nanocrystalline diamond interfaces." ASME 2020 IMECE, November 2020 (virtual).

176. **H. T. Aller**, X. Yu, A. Wise, R. Howell, A. Gellman, A. J. H. McGaughey, and J. A. Malen, "Thermal transport across Ga_2O_3/metal contact interfaces: Characterization and time-evolution." ASME 2020 IMECE, November 2020 (virtual).

175. **H.-Y. Kim** and A. J. H. McGaughey "Predicting phonon properties and thermal conductivity of rigid molecular crystals using rotational lattice dynamics." ASME 2020 IMECE, November 2020 (virtual).

174. **S. Zhang**, B. R. Jayan, and A. J. H. McGaughey, "Structure and energetics of point defects in titanium dioxide." MS&T20, November 2020 (virtual).

173. **J. Gong**, H.-Y. Kim, and A. J. H. McGaughey, "Neural network potential for lattice dynamics calculations and thermal conductivity prediction." MS&T20, November 2020 (virtual).

172. **S. Beltran**, W. Wang, A. J. H. McGaughey, P. R. LeDuc, and R. Taylor, "DNA nanostructures for mechanosensation." Society of Engineering Science Technical Meeting 2020, September 2020 (virtual).

171. **X. Wang**, Y. Li, J. A. Malen, A. J. H. McGaughey, "Assessing the Impact of Disjoining Pressure on Thin-Film Evaporation With Atomistic Simulation and Kinetic Theory." ASME Fluids Engineering Division Summer Meeting, July 2020 (virtual).

170. **X. Wang**, S. A. Ghaffarizadeh, A. J. H. McGaughey, and J. A. Malen, "Local Study of the Evaporation Mass Flux in Thin Liquid Films Using an Integrated Experimental and Computational Approach." ASME Fluids Engineering Division Summer Meeting, July 2020 (virtual).

169. **S. Zhang**, A. J. H. McGaughey, and R. Jayan, "Structure and energetics of point defects in titanium dioxide." 62nd Electronic Materials Conference, June 2020 (virtual).

168. **H. T. Aller**, N. Golio, K. Hobart, T. Feygelson, A. J. H. McGaughey, A. Gellman, and J. A. Malen, "Optimizing top-side device cooling via metal/nanocrystalline diamond Interfaces." 62nd Electronic Materials Conference, June 2020 (virtual).

167. **H. T. Aller**, X. Yu, K. Chabak, R. Howell, A. Gellman, A. J. H. McGaughey, and J. A. Malen, "Thermal transport across Ga_2O_3/metal contact interfaces: Characterization and time-Evolution." 62nd Electronic Materials Conference, June 2020 (virtual).

166. J. Gong, H.-Y. Kim, and **A. J. H. McGaughey**, "Neural network potential for lattice dynamics calculations and thermal conductivity prediction." NSF Workshop on Exuberance of Machine Learning in Transport Phenomena, Dallas, TX, February 2020.

165. **M. Bartnof**, Q. Liang, and A. J. H. McGaughey, "Predicting material properties of superatomic crystals using molecular dynamics simulations." MRS 2019 Fall Meeting, Boston, MA, December 2019.

164. G. Coloyan, B. P. Smith, K. D. Parrish, F. Wen, E. Fleming, K. Jarvis, A. J. H. McGaughey, E. Tutuc, and **L. Shi**, "Thermal conductivities and phonon mean free paths of silicon germanium nanowires of different lengths." MRS 2019 Fall Meeting, Boston, MA, December 2019.

163. **H. T. Aller**, Z. Guo, K. Hobart, T. I. Feygelson, A. J. H. McGaughey, A. Gellman, and J. A. Malen,"Thermal optimization of metal/nanocrystalline diamond junctions via diffusion barriers." MRS 2019 Fall Meeting, Boston, MA, December 2019.

162. **B. R. Jayan**, S. K. Jha, N. Nakamura, S. Zhang, L. Su, P. M. Smith, X. L. Phua, H. Wang, H. Wang, J. S. Okasinski, and A. J. H. McGaughey; "Defect-mediated anisotropic lattice expansion in ceramics as evidence for non-thermal coupling between electromagnetic fields and matter." MRS 2019 Fall Meeting, Boston, MA, December 2019.

161. **J. Han**, H. T. Aller, and A. J. H. McGaughey, "Impact of β-Ga_2O_3/Al_2O_3 lattice mismatch on interface structure and thermal transport." ASME 2019 IMECE, Salt Lake City, UT, November 2019.

160. **H. Parks**, V. Viswanathan, and A. J. H. McGaughey, "Uncertainty Quantification in First-Principles Predictions of Lattice Thermal Conductivity." 15th US National Congress on Computational Mechanics, Austin, TX, July 2019.

159. H. Parks, V. Viswanathan, and **A. J. H. McGaughey**, "Quantifying uncertainty in DFT predictions of the vibrational properties of molecules, molecular complexes, and crystals." Telluride Science Research Center workshop "Thermal Transport at the Nanoscale," June 2019.

158. **H.-Y. Kim**, B. Fu, K. D. Parrish, and A. J. H. McGaughey, "Phonon properties of confined thin films predicted from a two-dimensional lattice dynamics framework." MRS 2019 Spring Meeting, Phoenix, AZ, April 2019.

157. **J. A. Malen**, E. O'Brien, J. Russell, M. Bartnof, A. Christodoulides, K. Lee, D. Paley, A. J. H McGaughey, W.-L. Ong, X. Zhu, and X. Roy, "Orientational disorder controls the thermal conductivity of C_{70} based superatomic crystals." MRS 2019 Spring Meeting, Phoenix, AZ, April 2019.

156. **H. Aller**, J. A. Malen, and A. J. H. McGaughey, "Electron-phonon coupling in metal contacts - Two-temperature molecular dynamics simulations." MRS 2019 Spring Meeting, Phoenix, AZ, April 2019.

155. **H. Aller**, X. Yu, A. Wise, A. Gellman, A. J. H. McGaughey, and J. A. Malen, "Thermodynamically-driven oxidation at metal-β-Ga_2O_3 interfaces decreases their thermal boundary conductance." MRS 2019 Spring Meeting, Phoenix, AZ, April 2019.

154. H. L. Parks, V. Viswanathan, and **A. J. H. McGaughey**, "Uncertainty quantification of first-principles predictions of phonon dispersion and harmonic vibrational properties." MRS 2019 Spring Meeting, Phoenix, AZ, April 2019.

153. **J. Gong** and A. J. H. McGaughey, "Device-level thermodynamic model for an electrocaloric cooler." ASME 2018 IMECE, Pittsburgh, PA, November 2018.

152. **H. L. Parks**, V. Viswanathan, and A. J. H. McGaughey, "Quantifying uncertainty in first-principles predictions of phonon dispersion relations." ASME 2018 IMECE, Pittsburgh, PA, November 2018.

151. **M. Bartnof**, A. Christodoulides, W.-L. Ong, E. O'Brien, X. Roy, A. J. H. McGaughey, and J. A. Malen, "Fullerene-based Superatomic Crystals' Thermal Transport Controlled by Orientation Disorder." ASME 2018 IMECE, Pittsburgh, PA, November 2018.

150. **H. Aller**, X. Yu, A. Gellman, J. A. Malen, and A. J. H. McGaughey, "Thermal transport at Ga_2O_3/metal interfaces and bulk Ga_2O_3 polymorphs." ASME 2018 IMECE, Pittsburgh, PA, November 2018.

149. **X. Wang**, A. J. H. McGaughey, and J. A. Malen, "Local measurement of the evaporative heat transfer coefficient in thin films using frequency domain thermoreflectance" ASME 2018 IMECE, Pittsburgh, PA, November 2018.

148. **H.-Y. Kim** and A. J. H. McGaughey, "Mapping of phonon modes between two-dimensional and three-dimensional systems." ASME 2018 IMECE, Pittsburgh, PA, November 2018.

147. H. Aller, X. Yu, A. Gellman, J. A. Malen, and **A. J. H. McGaughey** "Thermal conductance of $\beta-Ga_2O_3$/metal interfaces." ITHERM 2018, San Diego, CA, May 2018.

146. **H. Babaei**, A. J. H. McGaughey, and C. E. Wilmer, "Transient mass and heat transfer during gas adsorption into MOFs." APS 2018 March Meeting, Los Angeles, CA, March 2018.

145. **J. A. Malen**, W.-L. Ong, E. O'Brien, G. Elbaz, D. Paley, C. F. Higgs III, A. J. H. McGaughey, and X. Roy, "Dynamic disorder controls thermal transport in superatomic crystals and organic-inorganic perovskites." MRS 2017 Spring Meeting, Phoenix, AZ, April 2017.

144. **H. Babaei**, A. J. H. McGaughey, and C. E. Wilmer, "Heat transfer in porous crystals containing adsorbed gases." MRS 2017 Spring Meeting, Phoenix, AZ, April 2017.

143. S. Majumdar, J. A. Malen, and **A. J. H. McGaughey**, "Cooperative molecular behavior enhances the thermal conductance of binary self-assembled monolayer junctions." MRS 2017 Spring Meeting, Phoenix, AZ, April 2017.

142. **K. D. Parrish**, J. Abel, A. Jain, J. A. Malen, and A. J. H. McGaughey, "Comparison of Monte Carlo methods for phonon-boundary scattering in nanoporous silicon films." MRS 2017 Spring Meeting, Phoenix, AZ, April 2017

141. **S. Kumar**, S. Lu, and A. J. H. McGaughey, "Degree-of-freedom resolved thermal transport in the C_{60} molecular crystal." MRS 2017 Spring Meeting, Phoenix, AZ, April 2017.

140. **F. Ramirez** and A. J. H. McGaughey, "Plasmon-induced hot electron generation in nanoparticle dimers." MRS 2017 Spring Meeting, Phoenix, AZ, April 2017.

139. **F. Ramirez**, S. Shen, and A. J. H. McGaughey, "Thermally Induced Surface Plasmons in Graphene Nanodisk Array." MRS 2016 Fall Meeting, Boston MA, November 2016.

138. **H. Babaei**, A. J. H. McGaughey, and C. E. Wilmer, "Heat Transfer in Metal Organic Frameworks during Gas Adsorption." 2016 AIChE Annual Meeting, San Francisco, CA, November 2016.

137. S. Majumdar, J. A. Malen, and **A. J. H. McGaughey**, "Thermal conductance of mixed self-assembled monolayer junctions." ASME 2016 IMECE, Phoenix, AZ, November 2016.

136. P. Thapar and **A. J. H. McGaughey**, "Negative thermal expansion in zeolites." ASME 2016 IMECE, Phoenix, AZ, November 2016.

135. S. Kumar, S. Lu, and **A. J. H. McGaughey**, "Mechanisms of thermal transport in C_{60} molecular crystals." ASME 2016 IMECE, Phoenix, AZ, November 2016.

134. **W.-L. Ong**, E. O'Brien, P. Dougherty, C. F. Higgs, III, A. J. H. McGaughey, X. Roy, and J. A. Malen, "Thermal conductivity of C_{60} superatom solids spans crystalline and amorphous behaviors." ASME 2016 IMECE, Phoenix, AZ, November 2016.

133. S. Majumdar, A. J. H. McGaughey, and **J. A. Malen**, "Mixed molecular layers create unique methods of thermal transport in organic-inorganic heterojunctions." ASME 2016 Summer Heat Transfer Conference, Washington, DC, July 2016.

132. **A. J. H. McGaughey**, "Thermal transport by phonons and electrons from first principles." Telluride Science Research Center workshop "Thermal Transport at the Nanoscale," June 2016.

131. **Y.-J. Yu** and A. J. H. McGaughey, "Electrocaloric cooling in PVDF-related ferroelectric polymers: First-passage kinetic Monte Carlo analysis." MRS 2016 Spring Meeting, Phoenix, AZ, March 2016.

130. **A. J. H. McGaughey** and Y.-J. Yu, "Multiscale modeling of the electrocaloric effect in PVDF-based polymers." APS 2016 March Meeting, Baltimore, MD, March 2016.

129. **S. Lu**, S, Kumar, and A. J. H. McGaughey, "Between crystal and glass: Thermal transport in C60 molecular crystals." APS 2016 March Meeting, Baltimore, MD, March 2016.

128. **S. Majumdar**, A. J. H. McGaughey, and J. A. Malen, "The role of molecular layer mixing on the thermal conductance of organic-inorganic heterojunctions." APS 2016 March Meeting, Baltimore, MD, March 2016.

127. **K. Parrish**, J. Freedman, K. Regner, A. Jain, J. A. Malen, and A. J. H. McGaughey, "Thermal conductivity accumulation function of silicon-germanium alloy from thermoreflectance and first-principles." APS 2016 March Meeting, Baltimore, MD, March 2016.

126. **W.-L. Ong**, E. O'Brien, P. Dougherty, J. , C. F. Higgs, III, X. Roy, A. J. H. McGaughey, and J. A. Malen, "Thermal conductivity behavior of superatom molecular crystals." APS 2016 March Meeting, Baltimore, MD, March 2016.

125. **J. A. Malen**, J. P Freedman, M. Jeong, J. Liang, X. Yu, S. Lu, A. J. H. McGaughey, A. Gellman, and J. A Bain, "Phonon transmission enhancement at metal-dielectric interfaces through adhesion layers and metal alloying." MRS 2015 Fall Meeting, Boston, MA, December 2015.

124. **S. Lu** and A. J. H. McGaughey, "Phonon transmission across supported Graphene-hBN interfaces." MRS 2015 Fall Meeting, Boston, MA, December 2015.

123. **K. Saaskilahti**, J. Oksanen, J. Tulkki, S, Volz, and A. J. H. McGaughey, "Spectral heat current distribution and phonon mean free path in amorphous silicon from non-equilibrium molecular dynamics." Phononics 2015, Paris, France, June 2015.

122. S. Lu and **A. J. H. McGaughey**, "Interplay of interference and anharmonicity in thermal transport across superlattice junctions." Phononics 2015, Paris, France, June 2015.

121. **Y.-J. Yu** and A. J. H. McGaughey, "Dipole-flipping energy barriers in PVDF-related ferroelectric polymers for electrocaloric cooling." 7th International Conference on Electroceramics, State College, PA, May 2015.

120. **A. Jain** and A. J. H. McGaughey, "Thermal transport by phonons and electrons in metals." MRS 2015 Spring Meeting, San Francisco, CA, April 2015.

119. **A. Jain** and A. J. H. McGaughey, "Strongly anisotropic in-plane thermal transport in single-layer black phosphorene." MRS 2015 Spring Meeting, San Francisco, CA, April 2015.

118. **S. Majumdar**, C. Mahoney, Z. Wang, C. M. Hui, M. N. Tchoul, K. Matyjaszewski, A. J.H. McGaughey, M. Bockstaller, and J. A. Malen, "Organic matrix interface effects on thermal transport in polymer nanocomposites." MRS 2015 Spring Meeting, San Francisco, CA, April 2015.

117. **S. Majumdar**, J. A. Sierra-Suarez, W.-L. Ong, C. F. Higgs, A. J.H. McGaughey, and J. A. Malen, "Controlling the thermal conductance of self-assembled monolayer junctions by tuning the vibrational alignment of the metal leads." MRS 2015 Spring Meeting, San Francisco, CA, April 2015.

116. W.-L. Ong, E. S. O'Brien, J. Epstein, A. J. H. McGaughey, X. Roy, and **J. A. Malen**, "Thermal conductivity of C_{60}-inorganic cluster molecular solids. MRS 2015 Spring Meeting, San Francisco, CA, April 2015.

115. **K. D. Parrish**, J. P. Freedman, J. A. Malen, and A. J. H. McGaughey, "Thermal conductivity accumulation in semiconductor alloys from thermoreflectance experiments and first-principles calculations." MRS 2015 Spring Meeting, San Francisco, CA, April 2015.

114. **C. S. Gorham** and A. J. H. McGaughey, "Thermal transport in C60 molecular crystals above room temperature." APS March Meeting 2015, San Antonio, TX, March 2015.

113. **A. Bhatti**, A. Jain, A. J. H. McGaughey, and N. Benedek, "Thermal transport properties of oxides from first principles." APS March Meeting 2015, San Antonio, TX, March 2015.

112. **Y.-J. Yu** and A. J. H. McGaughey, "Multiscale modeling of the electrocaloric effect in a P(VDF-TrFE-CFE) terpolymer." ASME 2014 IMECE, Montreal, PQ, November 2014.

111. **S. Majumdar**, S. Lu, A. Jain, J. A. Malen, and A. J. H. McGaughey, "Phonon mean free path-dependence of thermal interface conductance accumulation" ASME 2014 IMECE, Montreal, PQ, November 2014.

110. **K. T. Regner**, A. J. H. McGaughey, and J. A. Malen, "Relating frequency domain thermoreflectance thermal conductivity measurements to the accumulation function through an analytical solution to the Boltzmann transport equation submitted." ASME 2014 IMECE, Montreal, PQ, November 2014.

109. **S. Majumdar**, W. L. Ong, A. J. H. McGaughey, and J. A. Malen, "Debye temperature effect on thermal conductance across a self-assembled monolayer junction." ASME 2014 IMECE, Montreal, PQ, November 2014.

108. A. Jain and **A. J. H. McGaughey**, "Thermal conductivity of compound semiconductors: Interplay of density and acoustic-optical phonon dispersion gap." ASME 2014 IMECE, Montreal, PQ, November 2014.

107. **W. L Ong**, S. Rupich, E. O'Brien, J. Epstein, D. Talapin, X. Roy, A. J. H. McGaughey, and J. A. Malen, "Thermal conductivity of superatom molecular solids." 32nd International Thermal Conductivity Conference, West Lafayette, IN, April 2014.

106. **S. Majumdar**, A. Jain, S. Lu, J. A. Malen, and A. J. H. McGaughey, "Thermal interface conductance accumulation function." 32nd International Thermal Conductivity Conference, West Lafayette, IN, April 2014.

105. K. D. Parrish, **A. Jain**, J. M. Larkin, W. A. Saidi, and A. J. H. McGaughey, "Origins of thermal conductivity changes in strained systems." 32nd International Thermal Conductivity Conference, West Lafayette, IN, April 2014.

104. **A. Jain**, W. A. Saidi, and A. J. H. McGaughey, "First principles predictions of thermal conductivity of silicon and germanium." 32nd International Thermal Conductivity Conference, West Lafayette, IN, April 2014.

103. K. T. Regner, J. P. Freedman, J. M. Larkin, A. J. H. McGaughey, N. Abrosimov, S. Lubner, C. Dames, and **J. A. Malen**, "Phonon mean free path spectra measured by broadband frequency domain thermoreflectance." ASME 2013 IMECE, San Diego, CA, November 2013.

102. Y. Zhang, **Y. Wang**, and A. J. H. McGaughey, "Controlling lattice thermal conductivity via coherent phonon manipulation," ASME paper IMECE2013-65342. ASME 2013 IMECE, San Diego, CA, November 2013.

101. S. Majumdar, W. L. Ong, J. A. Malen, and **A. J. H. McGaughey**, "Atomistic mechanisms of thermal transport across organic-inorganic interfaces." ASME 2013 IMECE, San Diego, CA, November 2013.

100. S. Lu and **A. J. H. McGaughey**, "Phonon transport through multiple thin films." ASME 2013 IMECE, San Diego, CA, November 2013.

99. D. Guo, J. Gao, Y.-J. Yu, S. Santhanam, A. Slippey, G. K. Fedder, A. J. H. McGaughey, and S.-C. Yao, "Design of a fluid-based micro-scale electrocaloric refrigeration system," ASME paper HT2013-17396, ASME 2013 Summer Heat Transfer Conference, Minneapolis, MN, July 2013.

98. **S. C. Huberman**, J. M. Larkin, A. J. H. McGaughey, and C. H. Amon, "Effect of interspecies mixing on phonon mean free paths in superlattices." ASME 2013 Summer Heat Transfer Conference, Minneapolis, MN, July 2013.

97. J. M. Larkin and **A. J. H. McGaughey**, "Predicting vibrational mean free paths in disordered systems." ASME 2013 Summer Heat Transfer Conference, Minneapolis, MN, July 2013.

96. **K. Parrish**, J. M. Larkin, and A. J. H. McGaughey, "Origin of thermal conductivity changes in strained systems." ASME 2013 Summer Heat Transfer Conference, Minneapolis, MN, July 2013.

95. L. Hu and **A. J. H. McGaughey**, "Thermal accommodation of noble gases with single-walled carbon nanotubes." ASME 2013 Summer Heat Transfer Conference, Minneapolis, MN, July 2013.

94. J. M. Larkin and **A. J. H. McGaughey**, "Predicting vibrational mode properties in disordered systems," Telluride Science Research Center workshop "Thermal Transport at the Nanoscale," June 2013.

93. **W. L. Ong**, S. Rupich, D. Talapin, A. J. H. McGaughey, J. A. Malen, "Thermal conductivity measurements in hybrid organic-inorganic nanocrystal arrays." MRS 2013 Spring Meeting, San Francisco, CA, April 2013.

92. **K. Regner**, D. P. Sellan, J. P. Freedman, Z. Su, A. J. H. McGaughey, and J. A, Malen, "Phonon mean free path spectra measured by broadband frequency domain thermoreflectance." MRS 2013 Spring Meeting, San Francisco, CA, April 2013.

91. **S. Majumdar**, S. N. Schiffres, J. A. Malen, and A. J. H. McGaughey, "Dependence of thermal conductance of self-assembled monolayer junctions on physical properties and molecule chemistry." MRS 2013 Spring Meeting, San Francisco, CA, April 2013.

90. **A. Jain**, Y. J. Yu, and A. J. H. McGaughey, "Thermal conductivity of porous silicon films from first principles." MRS 2013 Spring Meeting, San Francisco, CA, April 2013.

89. **S. Lu** and A. J. H. McGaughey, "From single interface to superlattice: Phonon transport through systems of semiconductor thin films." MRS 2013 Spring Meeting, San Francisco, CA, April 2013.

88. **J. M. Larkin** and A. J. H. McGaughey, "Evaluation of the virtual crystal approximation for predicting thermal conductivity." MRS 2013 Spring Meeting, San Francisco, CA, April 2013.

87. **S. Majumdar**, S. N. Schiffres, J. A. Malen, and A. J. H. McGaughey, "Probing tunable thermal properties of organic hetero-junctions." APS 2013 March Meeting, Baltimore, MD, March 2013.

86. **W. L. Ong**, S. Rupich, D. Talapin, A. J. H. McGaughey, J. A. Malen, "Studies of thermal conductivity in hybrid organic-inorganic nanocrystal arrays." APS 2013 March Meeting, Baltimore, MD, March 2013.

85. **S. C. Huberman**, J. M. Larkin, A. J. H. McGaughey, and C. H. Amon, "Predicting phonon properties in superlattices from molecular dynamics and lattice dynamics." ASME 2012 IMECE, Houston, TX, November 2012. Second place (out of more then 200) in graduate student poster competition.

84. W. L. Ong, S. Rupich, D. Talapin, **A. J. H. McGaughey**, J. A. Malen, "Low temperature thermal conductivity measurements in nanocrystal superlattices." ASME 2012 IMECE, Houston, TX, November 2012.

83. S. Majumdar, J. A. Malen, and **A. J. H. McGaughey**, "Thermal transport in self-assembled monolayer junctions." ASME 2012 IMECE, Houston, TX, November 2012.

82. **S. Majumdar**, J. A. Malen, and A. J. H. McGaughey, "Characterizing thermal transport in self assembled monolayer junctions." 2012 AICHE Annual Meeting, Pittsburgh, PA, October 2012.

81. **W. L. Ong**, S. Rupich, D. Talapin, A. J. H. McGaughey, and J. A. Malen, "Studies of thermal conductivity in hybrid organic-inorganic nanocrystal superlattices." 2012 AICHE Annual Meeting, Pittsburgh, PA, October 2012.

80. **S. N. Schiffres**, L. Hu, K. H. Kim, M. I. Islam, A. J. H. McGaughey, and J. A. Malen, "Study of single-walled carbon nanotube aerogel thermal conductivity in the gas environment with varying aerogel density." 2012 AICHE Annual Meeting, Pittsburgh, PA, October 2012.

79. **D. Guo**, J. Gao, Y.-J. Yu, S. Santhanam, A. Slippey, G. K. Fedder, A. J. H. McGaughey, and S.-C. Yao, "Design of a fluid-based micro-scale electrocaloric refrigeration system," ASME paper HT2013-17396. ASME 2013 Summer Heat Transfer Conference, Minneapolis, MN, July 2013.

78. **J. M. Larkin** and A. J. H. McGaughey, "Ordered and disordered contributions to lattice thermal conductivity." Phonons 2012, Ann Arbor, MI, July 2012.

77. W. L. Ong, J. A. Malen, and **A. J. H. McGaughey**, "Atomistic modeling of heat transfer in hybrid organic-inorganic nanocrystal superlattices." ASME 2012 Summer Heat Transfer Conference, Puerto Rico, July 2012.

76. J. M. Larkin and **A. J. H. McGaughey**, "Ordered and disordered contributions to lattice thermal conductivity." ASME 2012 Summer Heat Transfer Conference, Puerto Rico, July 2012.

75. **A. Jain** and A. J. H. McGaughey, "Effect of phonon free path distributions on nanostructure thermal conductivity," ASME paper HT2012-58445. ASME 2012 Heat Transfer Conference, Puerto Rico, July 2012.

74. **D. Guo**, A. J. H. McGaughey, J. Gao, G. K. Fedder, M. Lee, and S.-C. Yao, "Numerical modeling of a micro-Stirling cooler," ASME paper HT2012-58361. ASME 2012 Heat Transfer Conference, Puerto Rico, July 2012.

73. **W.-L. Ong**, S. Rupich, D. Talapin, A. J. H. McGaughey, and J. A. Malen, "Thermal Conductivity of Hybrid Organic-Inorganic Nanocrystal Superlattices." ASME 2012 Micro/Nanoscale Heat and Mass Transfer International Conference, Atlanta, GA, March 2012.

72. **J. M. Larkin**, A. D. Massicotte, J. E. Turney, C. H. Amon, and A. J. H. McGaughey, "Comparison of spectral energy density methods for predicting phonon properties." ASME paper MNHMT2012-75071, ASME 2012 Micro/Nanoscale Heat and

Mass Transfer International Conference, Atlanta, GA, March 2012. **Honorable mention for best paper award.**

71. D. P. Sellan, V. Mishra, J. A. Malen, **A. J. H. McGaughey**, and C. H. Amon, "Assessment of Fourier-based thermal models used in frequency-domain thermoreflectance data analysis." ASME paper MNHMT2012-75087, ASME 2012 Micro/Nanoscale Heat and Mass Transfer International Conference, Atlanta, GA, March 2012.

70. **L. Hu**, H. Chen, G. Coloyan, and A. J. H. McGaughey, "Phonon transport in carbon nanotube aerogels." ASME paper MNHMT2012-75048, ASME 2012 Micro/Nanoscale Heat and Mass Transfer International Conference, Atlanta, GA, March 2012.

69. **J. M. Larkin** and A. J. H. McGaughey, "Predicting the Thermal Conductivity of Defected Systems Using the Spectral Energy Density." Fall 2011 MRS Meeting, Boston, MA, November 2011

68. **D. Guo**, J. Gao, A. J. H. McGaughey, M. Moran, S. Santhanam, G, K, Fedder, W. Anderson, and S.-C. Yao, "Design and evaluation of MEMS-based Stirling cycle microrefrigeration system," ASME paper IMECE2011-63084, ASME IMECE 2011, Denver, CO, November 2011.

67. T. E. Beechem, P. E. Hopkins, C. M. Reinke, M. F. Su, B. Kim, C. T. Harris, D. Goettler, M. Ziaei-Moayyed, E. A. Shaner, Z. C. Leseman, R. H. Olsson III, A. J. H. McGaughey, and **I. El-Kady**, "Thermal Conductivity Reduction in Phononic Crystals: Interplay of Coherent versus Incoherent Scattering." Phononics 2011, Santa Fe, NM, May 2011.

66. H. Chen and **A. J. H. McGaughey**, "Thermal transport through defected carbon nanotubes and carbon nanotube junctions." Spring 2011 MRS Meeting, San Francisco, CA, April 2011.

65. **A. V. Chernatynskyi**, P. Shukla, J. E. Turney, A. J. H. McGaughey, S. B. Sinnott, and S. R. Phillpot, "Thermal conductivity of ionic compounds: Applicability of the lattice dynamics and effects of the long range interactions." Spring 2011 MRS Meeting, San Francisco, CA, April 2011.

64. **D. P. Sellan**, E. S. Landry, J. E. Turney, A. J. H. McGaughey, and C. H. Amon, "System-size-effects in Green-Kubo and direct method molecular dynamics predictions of thermal conductivity." Spring 2011 MRS Meeting, San Francisco, CA, April 2011.

63. H. Chen and **A. J. H. McGaughey**, "Thermal conductivity of carbon nanotubes with defects." ASME paper AJTEC2011-44173, ASME/JSME 9th Thermal Engineering Joint Conference, Honolulu, HI, March 2011.

62. **A. J. H. McGaughey**, D. P. Sellan, E. S. Landry, and C. H. Amon, "Size-dependent model for thin film thermal conductivity." ASME paper AJTEC2011-44184, presented at 2011 ASME/JSME 9th Thermal Engineering Joint Conference, Honolulu, HI, March 2011.

61. J. E. Turney, J. A. Thomas, **A. J. H. McGaughey**, and C. H. Amon, "Predicting phonon properties from molecular dynamics simulation using the spectral energy density." ASME paper AJTEC2011-44315, 2011 ASME/JSME 9th Thermal Engineering Joint Conference, Honolulu, HI, March 2011.

60. **D. P. Sellan**, E. S. Landry, J. E. Turney, A. J. H. McGaughey, and C. H. Amon, "Size effects in Green-Kubo and direct method molecular dynamics predictions of thermal conductivity." ASME paper IMECE2010-38841, ASME IMECE 2010, Vancouver, BC, November 2010.

59. **M. Lee**, J. C. Yang , and A. J. H. McGaughey, "Cu(100) oxidation: Potential copper-releasing pathways for c(2x2) to missing row reconstruction transition." AVS 57th International Symposium and Exhibition, Albuquerque, NM, October 2010.

58. **D. P. Sellan**, J. E. Turney, E. S. Landry, A. J. H. McGaughey, and C. H. Amon, "Phonon Transport in Thin Films: A Lattice Dynamics/Boltzmann Transport Equation Study." ASME paper IHTC14-22623, International Heat Transfer Conference (IHTC-14), Washington DC, August 2010.

57. J. A. Thomas, R. M. Iutzi, J. E. Turney, C. H. Amon, and **A. J. H. McGaughey**, "Calculating the phonon properties of carbon nanotubes using the spectral energy density." ASME paper IHTC14-22262, International Heat Transfer Conference (IHTC-14), Washington DC, August 2010.

56. E. S. Landry and **A. J. H. McGaughey**, "Thermal transport across semiconductor interfaces and thin films." Third International Workshop on Transmission of Information and Energy in Nonlinear and Complex Systems, Singapore, July 2010.

55. **A. J. H. McGaughey**, "Predicting phonon properties using the spectral energy density." Thermal Transport at the Nanoscale workshop, Telluride Science Research Center, Telluride, CO, June 2010.

54. J. A. Thomas and **A. J. H. McGaughey**, "Predicting the phonon properties and thermal conductivity of carbon nanotubes using the spectral energy density." Spring 2010 MRS Meeting, April 2010, San Francisco, CA.

53. E. S. Landry and **A. J. H. McGaughey**, "Thermal resistance of semiconductor thin films predicted from lattice dynamics calculations and molecular dynamics simulations." ASME paper MNHMT2009-18341, ASME 2009 Micro/Nanoscale Heat and Mass Transfer International Conference, Shanghai, China, December 2009.

52. **M. Lee**, A. J. H. McGaughey, J. Ren, and J. C. Yang, "Investigation of oxygen embedment and surface reconstructuring on the Cu(100) surface by density functional theory calculations." AVS 56th International Symposium and Exhibition, San Jose, CA, November 2009.

51. J. A. Thomas and **A. J. H. McGaughey**, "Pressure driven water transport through single-walled carbon nanotubes." 2009 AIChE Annual Meeting, November 2009, Nashville, TN.

50. R. M. Iutzi, **E. S. Landry**, and A. J. H. McGaughey, "Thermal transport across a thin silica dielectric layer." Materials Science & Technology 2009, October 2009, Pittsburgh, PA.

49. **M. Lee**, A. J. H. McGaughey, J. Ren, and J. C. Yang, "Modeling early stages of Cu(100) oxidation by density functional theory." Materials Science & Technology 2009, October 2009, Pittsburgh, PA.

48. **J. Gu**, J. Melby, R. F. Davis, E. S. Landry, R. M. Iutzi, and A. J. H. McGaughey, "Breakdown mechanisms of thin SiO2 on Si(001)." Materials Science & Technology 2009, October 2009, Pittsburgh, PA.

47. **J. A. Thomas**, R. M. Iutzi, and A. J. H. McGaughey, "Thermal conductivity of water/carbon nanotube composite system." 30th International Thermal Conductivity Conference, September 2009, Pittsburgh, PA.

46. J. A. Thomas and **A. J. H. McGaughey**, "Effective thermal conductivity of CNT/water and graphene/water systems." ASME paper HT2009-88029, ASME 2009 Summer Heat Transfer Conference, San Francisco, CA, July 2009.

45. E. S. Landry and **A. J. H. McGaughey**, "Thermal resistance of silicon-germanium interfaces from lattice dynamics calculations." ASME paper HT2009-88025, ASME 2009 Summer Heat Transfer Conference, San Francisco, CA, July 2009.

44. **J. E. Turney**, A. J. H. McGaughey, and C. H. Amon, "Critically assessing the applicability of quantum corrections to classical thermal conductivity predictions." ASME paper HT2009-88129, ASME 2009 Summer Heat Transfer Conference, San Francisco, CA, July 2009.

43. **J. A. Thomas**, R. M. Iutzi, and A. J. H. McGaughey, "Water flow and heat transfer through carbon nanotube membranes: Insights from molecular dynamics simulations." 5th International Conference on Diffusion in Solids and Liquids, June 2009, Rome, Italy.

42. J. A. Thomas and **A. J. H. McGaughey**, "Thermal conductivity predictions of water/carbon nanotube composite systems." Spring 2009 MRS Meeting, April 2009, San Francisco, CA.

41. **E. S. Landry** and A. J. H. McGaughey, "Thermal resistance of semiconductor interfaces from lattice dynamics calculations." Spring 2009 MRS Meeting, April 2009, San Francisco, CA.

40. J. E.Turney, **A. J. H. McGaughey**, and C. H. Amon, "Investigation of phonon transport in superlattices by anharmonic lattice dynamics calculations." Spring 2009 MRS Meeting, April 2009, San Francisco, CA.

39. **C. Fleck**, J. Yang, A. H. McGaughey, and J, Ren, "KMC simulations in 3+1 dimensions and the effects of attachment probabilities and potential gradients on island morphologies." 2009 APS March Meeting, March 2009, Pittsburgh, PA.

38. **M. Lee**, A. J. H. McGaughey, S, Sinnott, S, Phillpot, and J, Yang, "Investigation of atomic oxygen embedment into copper surface by DFT calculation." 2009 APS March Meeting, March 2009, Pittsburgh, PA.

37. **J. A. Thomas** and A. J. H. McGaughey, "Water flow in carbon nanotubes: Transition from continuum to subcontinuum transport." 2009 APS March Meeting, March 2009, Pittsburgh, PA.

36. **E. S. Landry** and A. J. H. McGaughey, "Thermal boundary resistance of closely-spaced Si/Ge interfaces from lattice dynamics calculations." 2009 APS March Meeting, March 2009, Pittsburgh, PA.

35. **J. E.Turney**, A. J. H. McGaughey, and C. H. Amon, "Prediction of phonon transport properties and thermal conductivities by anharmonic lattice dynamic calculations." 2009 APS March Meeting, March 2009, Pittsburgh, PA.

34. E. S. Landry and **A. J. H. McGaughey**, "Atomistic modeling of thermal transport in realistic $Si/Si_{1-x}Ge_x$ superlattices." Fall 2008 MRS Meeting, December 2008, Boston, MA.

33. **M. Lee**, A. J. H. McGaughey, S. Sinnott, S. Phillpot, and J. Yang, "Modeling the early stages of copper oxidation by *ab initio* calculations." Fall 2008 MRS Meeting, December 2008, Boston, MA.

32. J. A. Thomas and **A. J. H. McGaughey**, "Mechanism of fast water transport through carbon nanotubes." 2008 APS Division of Fluid Dynamics Annual Meeting, November 2008, San Antonio, TX.

31. J. A. Thomas. O. Kuter-Arnebeck, and **A. J. H. McGaughey**, "Subcontinuum water transport through carbon nanotubes." 2008 APS Division of Fluid Dynamics Annual Meeting, November 2008, San Antonio, TX.

30. **J. A. Thomas** and A. J. H. McGaughey, "Identifying the mechanisms of enhanced water flow in carbon nanotubes." ASME paper IMECE2008-66489, ASME 2008 IMECE, Boston, MA, November 2008.

29. **E. S. Landry**, T. Matsuurra, and A. J. H. McGaughey, "Predicting the thermal boundary resistance of $Si/Si_{1-x}Ge_x$ isolated and closely-spaced interfaces with molecular dynamics simulations." ASME paper IMECE2008-67484, ASME 2008 IMECE, Boston, MA, November 2008.

28. **J. E. Turney**, A. J. H. McGaughey, and C. A. Amon, "Thin film thermal conductivity by anharmonic lattice dynamics calculations." ASME paper IMECE2008-66697, ASME 2008 IMECE, Boston, MA, November 2008.

27. E. S. Landry and **A. J. H. McGaughey**, "Designing $Si/Si_{1-x}Ge_x$ superlattices with tailored thermal transport properties." ASME paper HT2008-56473, ASME 2008 Summer Heat Transfer Conference, Jacksonville, FL, August 2008.

26. **J. E. Turney**, A. J. H. McGaughey, and C. Amon, "Argon thermal conductivity by anharmonic lattice dynamics calculations." ASME paper HT2008-56146, ASME 2008 Summer Heat Transfer Conference, Jacksonville, FL, August 2008.

25. **J. A. Thomas**, G. Jenness, A. J. H. McGaughey, and K. D. Jordan, "Water flow through carbon nanotubes and the water/carbon nanotube interaction potential." Many-Body Interactions: From Quantum Mechanics to Force Fields, Telluride, CO, July 2008.

24. **E. S. Landry**, T. Matsuurra, and A. J. H. McGaughey, "Molecular dynamics predictions of the thermal boundary resistance of isolated and closely-spaced $Si/Si_{1-x}Ge_x$ interfaces." Spring 2008 MRS Meeting, San Francisco CA, April 2008.

23. **E. S. Landry**, A. J. H. McGaughey, and M. I. Hussein, "Designing $Si/Si_{1-x}Ge_x$ Superlattices with Tailored Thermal Transport Properties." Spring 2008 MRS Meeting, San Francisco CA, April 2008.

22. **J. A. Thomas** and A. J. H. McGaughey, "Molecular dynamics simulation of water inside and outside carbon nanotubes." 2007 APS Division of Fluid Dynamics Annual Meeting, Salt Lake City, UT, November 2007.

21. **J. A. Thomas**, M. Paharia, E. S. Landry, G. Lee, and A. J. H. McGaughey, "Atomistic water droplet simulation." Presented at 2007 APS Division of Fluid Dynamics Annual Meeting, Salt Lake City, UT, November 2007.

20. E. S. Landry, **A. J. H. McGaughey**, and M. I. Hussein, "Molecular dynamics prediction of the thermal conductivity of Si/Si_xGe_{1-x} superlattices." ASME paper IMECE2007-43177, 2007 ASME IMECE, Seattle, WA, November 2007.

19. **B. Devine**, A. J. H. McGaughey, S. R. Phillpot, and S. B. Sinnott, "Molecular dynamics simulations of heteroepitaxial aluminum on α-aluminum oxide." AVS International Symposium and Exhibition, Seattle, WA, October 2007.

18. **B. Devine**, A. J. H. McGaughey, S. R. Phillpot, and S. B. Sinnott, "Computational study of the interfacial structure of aluminum/α-alumina." 2007 International Workshop on Synthesis of Functional Oxide Materials, Santa Barbara, CA, August 2007.

17. **E. S. Landry**, A. J. H. McGaughey, and M. I. Hussein, "Molecular dynamics prediction of the thermal conductivity of Si/Ge superlattices." ASME paper HT2007-32152, ASME 2007 Summer Heat Transfer Conference, Vancouver, BC, July 2007.

16. S. Mikkilineni, **E. S. Landry**, and A. J. H. McGaughey, "Subcritical and supercritical nanodroplet evaporation: A molecular dynamics study." ASME paper HT2007-32418, ASME 2007 Summer Heat Transfer Conference, Vancouver, BC, July 2007.

15. **J. E. Turney**, A. J. H. McGaughey, and C. Amon "Effects of confinement and surface relaxation on the lattice dynamics and thermal transport properties of thin films." ASME paper HT2007-32274 ASME 2007 Summer Heat Transfer Conference, Vancouver, BC, July 2007.

14. E. S. Landry, S. Mikkilineni, and **A. J. H. McGaughey**, "Subcritical and supercritical nanodroplet evaporation: A molecular dynamics study." ILASS Americas 20th Annual Conference on Liquid Atomization and Spray Systems, Chicago, IL, May 2007.

13. **S. Shenogin**, A. Bodapati, A. J. H. McGaughey, and P. Keblinski, "Thermal transport mechanism in inorganic and polymeric glasses." MRS 2007 Spring Meeting, San Francisco, CA, April 2007.

12. **A. J. H. McGaughey** "Charge transfer potential for copper-oxygen systems," 2nd Meeting on Reactive Potential Development, Gainesville, FL, January 2007.

11. **B. Devine**, A. J. H. McGaughey, S. R. Phillpot, and S. B. Sinnott, "Development of an efficient charge transfer potential for the molecular dynamics study of metal/metal oxide interfaces." AVS International Symposium and Exhibition, San Francisco, CA, November 2006.

10. **J. A. Thomas** and A. J. H. McGaughey, "Effect of surface wettability on liquid structure and mobility near a solid surface." 2006 APS Division of Fluid Dynamics Annual Meeting, Tampa Bay, FL, November 2006.

9. **E. S. Landry** and A. J. H. McGaughey, "Superlattice analysis for tailored thermal transport characteristics." ASME paper IMECE2006-13673, IMECE 2006, Chicago, IL, November 2006.

8. **A. J. H. McGaughey** and J. Li, "Molecular dynamics prediction of the thermal resistance of solid-solid interfaces in superlattices." ASME paper IMECE2006-13590, IMECE 2006, Chicago, IL, November 2006.

7. **B. Devine**, A. J. H. McGaughey, S. R. Phillpot, and S. B. Sinnott, "Molecular dynamics simulation of the (111) aluminum/(0001) α-aluminum oxide." AVS International Symposium and Exhibition, Boston, MA, November 2005.

6. **A. J. H. McGaughey**, S. R. Phillpot, S. B. Sinnott, and J. Yang, "Multiscale simulation of copper oxidation." Materials Science & Technology 2005, Pittsburgh, PA, September 2005.

5. A. J. H. McGaughey, **M. I. Hussein**, M. Kaviany, and G. Hulbert, "Phonon band structure and thermal transport correlation in a two-atom unit cell." ASME paper IMECE2004-62328, 2004 ASME IMECE, Anaheim, CA, November 2004.

4. **A. J. H. McGaughey** and M. Kaviany, "Nature of phonon transport in molecular dynamics simulations." APS Spring Meeting, Montreal, PQ, March 2004.

3. **A. J. H. McGaughey**, J. D. Chung, and M. Kaviany, "Integration of molecular dynamics simulations and Boltzmann transport equation in phonon thermal conductivity analysis." ASME paper IMECE2003-41899, 2003 ASME IMECE, Washington, DC, November 2003.

2. **A. J. H. McGaughey** and M. Kaviany, "Molecular dynamics calculations of the thermal conductivity of silica based crystals." AIAA paper 2002-3343, 8th AIAA/ASME Joint Thermophysics and Heat Transfer Conference, St. Louis, MO, June 2002.

1. **A. J. H. McGaughey** and C. A. Ward, "Stable droplets in finite volumes." 15th International Conference on Nucleation and Atmospheric Aerosols, Rolla, MO, August 2000.