

Curriculum Vitae

Dr. Ming Hu

Associate Professor
Department of Mechanical Engineering
University of South Carolina
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• Research Interests

Micro-/Nano-scale Thermal Transport • Energy Materials • Energy Conversion and Energy Nanotechnology • Multi-scale Simulation of Thermal Transport and Materials Processing • Phase Change Materials • Thermal Management

• Education

2001.9 - 2007.3 Doctor of Engineering in mechanics from Institute of Mechanics, Chinese Academy of Sciences, in Beijing, China

1997.9 - 2001.7 Bachelor of Science in theoretical and applied mechanics from Department of Modern Mechanics, University of Science and Technology of China, in Hefei City, Anhui Province, China

• Employment

2018.3 - present Associate Professor in Department of Mechanical Engineering, University of South Carolina, Columbia, SC, USA

2013.2 - 2018.2 Assistant Professor in Institute of Mineral Engineering, Faculty of Georesources and Materials Engineering, RWTH Aachen University, in Aachen, Germany

2009.1 - 2013.2 Senior Research Scientist in Laboratory of Thermodynamics in Emerging Technologies, Department of Mechanical and Process Engineering, Swiss Federal Institute of Technology (ETH) Zurich, in Zurich, Switzerland

2006.9 - 2009.1 Postdoctoral Research Associate in Nanoscale Science and Engineering Center, Department of Material Science and Engineering, Rensselaer Polytechnic Institute, in Troy, NY, USA

• Fellowships and Awards

2014 Theodore von Kármán Fellowship, RWTH Aachen University
2005 Presidential Fellowship, Chinese Academy of Sciences

- 2005 Guo Yonghuai Fellowship, Institute of Mechanics, CAS
- 2005 Outstanding Student Scholarship (Grade 1), Institute of Mechanics, CAS
- 2004 Outstanding Student Scholarship (Grade 2), Institute of Mechanics, CAS
- 2002 Outstanding Graduate Scholarship, Graduate School, CAS
- 2000 Outstanding Student Scholarship (Grade 3), USTC
- 1999 Outstanding Student Scholarship (Grade 2), USTC
- 1998 Outstanding Student Scholarship (Grade 3), USTC

• Professional Activities

University-Level Teaching

Bachelor-level course:

“Introduction to Mechanics of Solids”, fall semester 2018, University of South Carolina
 “Computer Simulation of Materials”, winter semester 2013 / 2014 / 2015 / 2016 / 2017, RWTH Aachen University

Master-level courses:

“Transport Phenomena I”, winter semester 2016 / 2017, RWTH Aachen University
 “Transport Phenomena II”, summer semester 2017, RWTH Aachen University
 “Thermophysics of Low-dimensional Materials”, summer semester 2017, RWTH Aachen University
 “Introduction to Molecular Simulation”, summer semester 2016, RWTH Aachen University
 “Introduction to Molecular Dynamics Simulation”, winter semester 2013 / 2014 / 2015 / 2016 / 2017, RWTH Aachen University
 “Computational Materials Science”, winter semester 2014 / 2015 / 2016 / 2017, RWTH Aachen University
 “Fundamentals of Materials Interface and Interface Engineering”, summer semester 2015 / 2016 / 2017, RWTH Aachen University
 “Principles and Engineering Applications of Molecular Dynamics Simulations”, fall semester 2010 / 2011 / 2012, ETH Zurich

Organization of International Scientific Meetings

2017 Symposium co-organizer, E-MRS Spring Meeting, Strasbourg, France
 2016 Session chair, EMN Meeting on Nanowires, Amsterdam, Netherlands
 2016 Session chair, EMN Meeting on Thermoelectric Materials, Orlando, FL, US
 2015 Session co-chair, “ASME 2015 International Mechanical Engineering Congress and Exposition” (IMECE), Houston, US
 2015 Conference organizer, “3rd European Community of Computational Methods in Applied Sciences (ECCOMAS) Young Investigators Conferences” (YIC), Aachen, Germany
 2014 Topic organizer, “ASME 2014 International Mechanical Engineering Congress and Exposition” (IMECE), Montreal, Canada
 2014 Symposium organizer, “International Conference on Computational and Experimental Engineering and Sciences” (ICCES’14), Changwon, Korea

Journal Reviewers (280+ times in total)

AIP Advances; Applied Materials & Interfaces; APL Materials; Applied Physics A; Applied Physics Letters; Applied Thermal Engineering; Carbon; Chemical Physics Letters; Chemistry of Materials; Colloids and Surfaces A; Colloids and Surfaces D; Computational Materials Science; Continuum Mechanics and Thermodynamics; Central European Journal of Physics; EPL; International Journal of Heat and Mass Transfer; International Journal of Thermal Sciences; Journal of Applied Physics; Journal of Chemical Physics; Journal of Computational Physics; Journal of Crystal Growth; Journal of Heat Transfer; Journal of Materials Chemistry A; Journal of Materials Chemistry C; Journal of Nanoparticle Research; Journal of Non-Crystalline Solids; Journal of Physical Chemistry C; Journal of Physical Chemistry Letters; Journal of Physics: Condensed Matter; Journal of Physics D: Applied Physics; Lab on a Chip;

Materials and Design; Molecular Physics; Nano Energy; Nano Research; Nanomaterials and Nanotechnology; Nanoscale; Nanoscale and Microscale Thermophysical Engineering; Nanotechnology; Nano Letters; Nature; Nature Communications; Nature Physics; Physica E; Physica Status Solidi A: Applications and Materials Science; Physica Status Solidi B: Basic Solid State Physics; Physical Chemistry Chemical Physics; Physical Review B; Physical Review Letters; Physical Review Materials; Recent Patents on Nanotechnology; RSC Advances; RSC Analytical Methods; Scientific Reports; Scripta Materialia; Small; Ultramicroscopy; Vacuum

Editorial Membership

Editorial board member: Scientific Reports (Nature Publishing Group)

Guest editor: Materials (special issue on “*Thermal Sciences and Thermodynamics of Materials*”)

Topic editor: Frontiers in Physics (Research Topic on “*Computer Modelling of Micro - and Nano - scale Thermal Transport and its Application in Emerging Energy Nanotechnologies*”)

• **Publications**

○ **Books and book chapters**

4. **Ming Hu**, Hua Bao, and Yaping Dan, Book chapter “Si nanowires for evolutionary nanotechnology”, in book “Silicon Nanomaterials Sourcebook - Low-Dimensional Structures Nanopowders, Nanowires”, edited by Klaus D. Sattler, CRC Press, 2017

3. Guangzhao Qin, Han Xie, **Ming Hu**, and Hua Bao, Book chapter “Two-dimensional silicon”, in book “Silicon Nanomaterials Sourcebook - Low-Dimensional Structures Nanopowders, Nanowires”, edited by Klaus D. Sattler, CRC Press, 2017

2. Guangzhao Qin and **Ming Hu**, Book chapter “Diverse Thermal Transport Properties of Two-Dimensional Materials: A Comparative Review”, in book “Two-dimensional Materials: Synthesis, Characterization and Potential Applications”, edited by Pramoda Nayak, InTech, 2016

1. **Ming Hu**, Book chapter “Atomistic Modeling of Nanostructured Materials for Novel Energy Application”, in book “Modeling, Characterization, and Production of Nanomaterials”, edited by Vinod Tewary and Yong Zhang, Elsevier, 2015

○ **Peer-reviewed journal papers (* corresponding author, total citations: ~2900+, H-index: 31, as of 12/02/2018)**

119. Jun Zhang, Chaowei Li, Cuiping Yu, Xiaona Wang, Qiulong Li, Huifen Lu, Qichong Zhang, Jingxin Zhao, Songfeng E, **Ming Hu**, Yagang Yao,* "Large Improvement of Thermal Transport and Mechanical Performance of Polyvinyl Alcohol Composites Based on Interface Enhanced by SiO₂ Nanoparticle-Modified-Hexagonal Boron Nitride", *Composites Science and Technology*, **169**, 167 (2019).

118. Yufei Gao,* Xiaoliang Zhang,* Dawei Tang, and **Ming Hu**,* "Unexpected Anisotropy of (14,14,14)-Graphyne: a Comprehensive Study on the Thermal Transport Properties of Graphyne Based Nanomaterials", *Carbon*, **143**, 189 (2019).

117. Yanguang Zhou,* Shiyun Xiong,* Xiaoliang Zhang, Sebastian Volz,* and **Ming Hu**,* "Thermal Transport Crossover from Crystalline to Partial-Crystalline Partial-Liquid State", *Nature Communications*, **9**, 4712 (2018).

116. Sheng-Ying Yue, Cheng Long, Bolin Liao,* and **Ming Hu**,* "Electron-Phonon Interaction and Superconductivity in the High-Pressure cI16 Phase of Lithium from

First-Principles", *Physical Chemistry Chemical Physics*, **20**, 27125 (2018).

115. Kunpeng Yuan, Xiaoliang Zhang,* Dawei Tang,* and Ming Hu,* "Anomalous Pressure Effect on the Thermal Conductivity of ZnO, GaN, and AlN from First-Principles Calculations", *Physical Review B*, **98**, 144303 (2018).

114. Biyao Wu, Yanguang Zhou, and Ming Hu,* "Two Channels Thermal Transport in Ordered-Disordered Superionic Ag₂Te and its Traditionally Contradictory Enhancement by Nanotwin Boundary", *Journal of Physical Chemistry Letters*, **9**, 5704 (2018).

113. Yufei Gao, Yanguang Zhou, and Ming Hu,* "Enormous Suppression of Phonon Transport in Silicon Nanowires with Five-Fold Twin Boundary", *Journal of Materials Chemistry A*, **6**, 18533 (2018).

112. Jia-Yue Yang and Ming Hu,* "Strong Electron-Phonon Interaction Retarding Phonon Transport in Superconducting Hydrogen Sulfide (H₃S) at High Pressures", *Physical Chemistry Chemical Physics*, **20**, 24222 (2018).

111. Xin He, Zehui Zhang, Chenhui Zhang, Yang Yang, Ming Hu, Weikun Ge, and Xixiang Zhang,* "Exploration of Exciton Behavior in Atomically Thin WS₂ Layers by Ionic Gating", *Applied Physics Letters*, **113**, 013104 (2018).

110. Chengxiao Peng, Guangzhao Qin, Lichuan Zhang, Guangbiao Zhang, Chao Wang, Yuli Yan, Yuanxu Wang,* and Ming Hu,* "Dependence of Phonon Transport Properties with Stacking Thickness in Layered ZnO", *Journal of Physics D: Applied Physics*, **51**, 315303 (2018).

109. Guangzhao Qin, Zhenzhen Qin, Huimin Wang, and Ming Hu,* "Lone-Pair Electrons Induced Anomalous Enhancement of Thermal Transport in Strained Planar Two-Dimensional Materials", *Nano Energy*, **50**, 425 (2018).

108. Chengxiao Peng, Guangbiao Zhang, Chao Wang, Yuli Yan, Haiwu Zheng, Yuanxu Wang,* and Ming Hu,* "Improvement of Thermoelectricity through Magnetic Interactions in Layered Cr₂Ge₂Te₆", *Physica Status Solidi (RRL) - Rapid Research Letters*, (DOI: 10.1002/pssr.201800172).

107. Zhenzhen Qin, Guangzhao Qin,* and Ming Hu,* "Origin of Anisotropic Negative Poisson's Ratio in Graphene", *Nanoscale*, **10**, 10365 (2018)

106. Guangzhao Qin, Zhenzhen Qin, Huimin Wang, and Ming Hu,* "On the Diversity in the Thermal Transport Properties of Graphene: A First-Principles-Benchmark Study Testing Different Exchange-Correlation Functionals", *Computational Materials Science*, **151**, 153 (2018).

105. Huimin Wang, Guangzhao Qin, Zhenzhen Qin, Guojian Li, Qiang Wang,* and Ming Hu,* "Lone-pair Electrons do not Necessarily Lead to Low Lattice Thermal Conductivity: an Exception of Two-dimensional Penta-CN₂", *Journal of Physical Chemistry Letters*, **9**, 2474 (2018).

104. Zhi Liang* and Ming Hu,* "Tutorial: Determination of Thermal Boundary Resistance by Molecular Dynamics Simulations", *Journal of Applied Physics*, **123**, 191101 (2018).

103. Yufei Gao, Yanguang Zhou, Xiaoliang Zhang,* and Ming Hu,* "Extremely Low Thermal Conductivity of Polycrystalline Silicene", *Journal of Physical Chemistry C*, **122**, 9220 (2018).

102. Cuiping Yu, Wenbin Gong, Wei Tian,* Qichong Zhang, Yancui Xu, Ziyin Lin, **Ming Hu**, Xiaodong Fan, and Yagang Yao,* "Hot-pressing Induced Alignment of Boron Nitride in Polyurethane for Composite Films with Thermal Conductivity over $50 \text{ Wm}^{-1} \text{ K}^{-1}$ ", *Composites Science and Technology*, **160**, 199 (2018).
101. Yupeng Shen, Fancy Qian Wang, Jie Liu, Yaguang Guo, Xiaoyin Li, Guangzhao Qin, **Ming Hu**, and Qian Wang,* "A C20 fullerene-based sheet with ultrahigh thermal conductivity", *Nanoscale*, **10**, 6099 (2018).
100. Yang Han, Jia-Yue Yang, and **Ming Hu**,* "Unusual Strain Response of Thermal Transport in Dimerized Three-Dimensional Graphene", *Nanoscale*, **10**, 5229 (2018).
99. Yanguang Zhou,* Jia-Yue Yang, Long Cheng, and **Ming Hu**,* "Strong Anharmonic Phonon Scattering Induced Giant Reduction of Thermal Conductivity in PbTe Nanotwin Boundary", *Physical Review B*, **97**, 085304 (2018).
98. Yanguang Zhou, Zheyong Fan, Guangzhao Qin, Jia-Yue Yang, Tao Ouyang, and **Ming Hu**,* "Methodology Perspective of Computing Thermal Transport in Low-dimensional Materials and Nanostructures: the Old and the New", *ACS Omega*, **3**, 3278 (2018). **Invited Perspective**
97. Xufei Wu, Vikas Varshney, Jonghoon Jay Lee, Guangzhao Qin, **Ming Hu**, Ajit Roy, and Tengfei Luo,* "Bond Saturation Significantly Enhances Thermal Energy Transport in Two-Dimensional Pentagonal Materials", *Nano Energy*, **45**, 1 (2018).
96. Guangzhao Qin and **Ming Hu**,* "Accelerating Evaluation of Converged Lattice Thermal Conductivity", *NPJ Computational Materials*, **4**, 3 (2018).
95. Jia-Yue Yang, Long Cheng, and **Ming Hu**,* "Unravelling the Progressive Role of Rattlers in Thermoelectric Clathrate and Strategies for Performance Improvement: Concurrently Enhancing Electronic Transport and Blocking Phononic Transport", *Applied Physics Letters*, **111**, 242101 (2017).
94. Guangzhao Qin and **Ming Hu**,* "Thermal Transport in Phosphorene", *Small*, 1702465 (2018). **Invited Review**
93. Jian Han, Ben Xu,* **Ming Hu**, Y.-H. Lin, and W. Liu, "Analytical Study on the Size Effect of Phonon Spectral Energy Density Resolution", *Computational Materials Science*, **132**, 6 (2017).
92. Huimin Wang, Guangzhao Qin, Guojian Li, Qiang Wang,* and **Ming Hu**,* "Unconventional Thermal Transport Enhancement with Large Atom Mass: a Comparative Study of Two-dimensional Transition Dichalcogenides", *2D Materials*, **5**, 015022 (2018).
91. Cheng Shao, Qingyuan Rong, **Ming Hu**, and Hua Bao,* "Probing the Phonon Surface Interaction by Wave Packet Simulation: Effect of Roughness and Morphology", *Journal of Applied Physics*, (accepted).
90. Benhu Zhou,* Yufei Gao, Benliang Zhou, Yagang Yao, Guanghui Zhou,* and **Ming Hu**,* "Enhanced thermoelectric properties of the AGNR-GYNR heterojunctions", *Physics Letters A*, **381**, 3766 (2017).
89. Yufei Gao, Xiaoliang Zhang, Yanguang Zhou and **Ming Hu**,* "Giant Reduction in Thermal Conductivity of Extended Type-I Silicon Clathrates and Prominent Thermal Effect of 6d Guest Wyckoff Positions", *Journal of Materials Chemistry C*, **5**, 10578 (2017).

88. Jun Zhang, Xiaona Wang, Cuiping Yu, Qiulong Li, Zhuo Li, * Chaowei Li, Huifen Lu, Qichong Zhang, Jingxin Zhao, **Ming Hu** and Yagang Yao, * "A Facile Method to Prepare Flexible Boron Nitride/poly(vinyl alcohol) Composites with Enhanced Thermal Conductivity", *Composites Science and Technology*, **149**, 41 (2017).
87. Guangzhao Qin and **Ming Hu**, * "Thermal Transport Properties of Monolayer Phosphorene: a Mini-review of Theoretical Studies", *Frontiers in Energy*, (accepted).
86. Yanguang Zhou, * Xiaojing Gong, Ben Xu and **Ming Hu**, * "First-Principles and Molecular Dynamics Study of Thermoelectric Transport Properties of N-type Silicon-based Superlattice-Nanocrystalline Heterostructures", *Journal of Applied Physics*, **122**, 085105 (2017).
85. Jia-Yue Yang and **Ming Hu**, * "Temperature Induced Large Broadening and Blueshift in the Electronic Band Structure and Optical Absorption of Methylammonium Lead Iodide Perovskite", *Journal of Physical Chemistry Letters*, **8**, 3720 (2017).
84. Huifen Lu, Jun Zhang, Jie Luo, Wenbin Gong, Chaowei Li, Qiulong Li, Kai Zhang, **Ming Hu**, Yagang Yao, * "Enhanced Thermal Conductivity of Free-Standing 3D Hierarchical Carbon Nanotube-Graphene Hybrid Paper", *Composites Part A*, **102**, 1 (2017).
83. Benhu Zhou, * Benliang Zhou, Yagang Yao, Guanghui Zhou, * and **Ming Hu**, * "Spin-dependent Seebeck Effects in a Graphene Superlattice p-n Junction with Different Shapes", *Journal of Physics: Condensed Matter*, **29**, 405303 (2017).
82. Long Cheng, Qing-Bo Yan, * and **Ming Hu**, * "Role of Phonon-phonon and Electron-phonon Scattering in Thermal Transport in PdCoO₂", *Physical Chemistry Chemical Physics*, **19**, 21714 (2017).
81. Yang Han, Yanguang Zhou, Guangzhao Qin, Jinming Dong, Douglas S. Galvao, and **Ming Hu**, * "Unprecedented Mechanical Response of the Lattice Thermal Conductivity of Auxetic Carbon Crystals", *Carbon*, **122**, 374 (2017).
80. Yanguang Zhou, Xiaojing Gong, Ben Xu, and **Ming Hu**, * "Decouple Electronic and Phononic Transport in Nanotwinned Structure: A New Strategy for Enhancing the Figure-of-merit of Thermoelectrics", *Nanoscale*, (published online).
79. Guangzhao Qin, Zhenzhen Qin, Sheng-Ying Yue, Qing-Bo Yan, and **Ming Hu**, * "External Electric Field Driving Ultra-low Thermal Conductivity of Silicene", *Nanoscale*, **9**, 7227 (2017).
78. Guangzhao Qin, Zhenzhen Qin, Huimin Wang, and **Ming Hu**, * "Anomalous Temperature-dependent Thermal Conductivity of Monolayer GaN with Large Deviations from the Traditional 1/T Law", *Physical Review B*, **95**, 195416 (2017).
77. Sheng-Ying Yue, Xiaoliang Zhang, Guangzhao Qin, Simon R. Phillpot, * and **Ming Hu**, * "A Metric for Strong Intrinsic Fourth-Order Phonon Anharmonicity", *Physical Review B*, **95**, 195203 (2017).
76. Hui-Min Wang, Guangzhao Qin, Guojian Li, Qiang Wang, * and **Ming Hu**, * "Low Thermal Conductivity of Monolayer ZnO and its Anomalous Temperature Dependence", *Physical Chemistry Chemical Physics*, **19**, 12882 (2017).
75. Yanguang Zhou and **Ming Hu**, * "Full Quantification of Frequency Dependent Interfacial Thermal Conductance Contributed by Two- and Three-phonon Scattering

Process from Non-Equilibrium Molecular Dynamics Simulation”, *Physical Review B*, **95**, 115313 (2017).

74. Zhenzhen Qin, Guangzhao Qin, Xu Zuo,* Zhihua Xiong,* and **Ming Hu**,* “Orbitally Driven Low Thermal Conductivity of Monolayer Gallium Nitride (GaN) with Planar Honeycomb Structure: a Comparative Study”, *Nanoscale*, **9**, 4295 (2017).

73. Sheng-Ying Yue, Guangzhao Qin, Xiaoliang Zhang, Xianlei Sheng, Gang Su,* and **Ming Hu**,* “Thermal Transport in Novel Carbon Allotropes with sp^2 or sp^3 Hybridization: an *Ab Initio* Study”, *Physical Review B*, **95**, 085207 (2017).

72. Yanguang Zhou, Xiaoliang Zhang, and **Ming Hu**,* “Nonmonotonic Diameter Dependence of Thermal Conductivity of Extremely Thin Si Nanowires: Competition between Hydrodynamic Phonon Flow and Boundary Scattering”, *Nano Letters*, **17**, 1269 (2017).

71. Huachao Yang, Xiaoliang Zhang, Jinyuan Yang, Zheng Bo,* **Ming Hu**,* Jianhua Yan, and Kefa Cen, “Molecular Origin of Electric Double-Layer Capacitors at Multilayer Graphene Edges”, *Journal of Physical Chemistry Letters*, **8**, 153 (2017).

70. Yanguang Zhou* and **Ming Hu**,* “Mechanical Behaviors of Nanocrystalline Cu/SiC Composites: an Atomistic Investigation”, *Computational Materials Science*, **129**, 129 (2017).

69. Tao Ouyang,* Huaping Xiao, Chao Tang, Xiaoliang Zhang, **Ming Hu**,* and Jianxin Zhong, “First-principles Study of Thermal Transport in Nitrogenated Holey Graphene”, *Nanotechnology*, **28**, 045709 (2017).

68. Jia-Yue Yang, Sheng-Ying Yue, and **Ming Hu**,* “Bidirectional Effect of Magnetic Field on Electronic Thermal Transport of Metals from All-Electron First-Principles Calculations”, *Physical Review B*, **94**, 235153 (2016).

67. Jia-Yue Yang, Guangzhao Qin, and **Ming Hu**,* “Nontrivial Contribution of Fröhlich Electron-Phonon Interaction to Lattice Thermal Conductivity of Wurtzite GaN”, *Applied Physics Letters*, **109**, 242103 (2016).

66. Guangzhao Qin, Xiaoliang Zhang, Sheng-Ying Yue, Zhenzhen Qin, Huimin Wang, Yang Han, and **Ming Hu**,* “Resonant Bonding Driven Giant Phonon Anharmonicity and Low Thermal Conductivity of Phosphorene”, *Physical Review B*, **94**, 165445 (2016).

65. Xiaoliang Zhang, Xiaojing Gong, Yanguang Zhou, and **Ming Hu**,* “Tailoring Thermal Conductivity of AlN Films by Periodically Aligned Surface Nano-grooves”, *Applied Physics Letters*, **109**, 133107 (2016).

64. Sheng-Ying Yue, Xiaoliang Zhang, Guangzhao Qin, Jiayue Yang, and **Ming Hu**,* “Insight into the Collective Vibrational Modes Driving Ultra-low Thermal Conductivity of Perovskite Solar Cells”, *Physical Review B*, **94**, 115427 (2016).

63. Yanguang Zhou and **Ming Hu**,* “Record Low Thermal Conductivity of Polycrystalline Si Nanowire: Breaking the Casimir Limit by Severe Suppression of Propagons”, *Nano Letters*, **16**, 6178 (2016).

(Featured on Phys.org: <http://phys.org/news/2016-10-thermoelectric-silicon-material-record-low-thermal.html>)

62. Ying Pan, Ye Tao, Guangzhao Qin, Yuriy Fedoryshyn, Shyamprasad N. Raja, **Ming Hu**, Christian L. Degen, and Dimos Poulikakos,* “Surface Chemical Tuning of Phonon and Electron Transport in Free-Standing Silicon Nanowire Arrays”, *Nano Letters*, **16**,

6364 (2016).

61. Sheng-Ying Yue, Xiaoliang Zhang, Stephen Stackhouse, Guangzhao Qin, Edoardo Di Napoli, and Ming Hu,* "Methodology for Determining the Electronic Thermal Conductivity of Metals via Direct Non-Equilibrium Ab Initio Molecular Dynamics", *Physical Review B*, **94**, 075149 (2016).

60. Yang Han, Jinming Dong, Guangzhao Qin, and Ming Hu,* "Phonon Transport in Ground State of Two-dimensional Silicon and Germanium", *RSC Advances*, **6**, 69956 (2016).

59. Guo Hong, Yang Han, Thomas M. Schutzius, Yuming Wang, Ying Pan, Ming Hu, Jiansheng Jie, Chander S. Sharma, Ulrich Müller, and Dimos Poulidakos,* "On the Mechanism of Hydrophilicity of Graphene", *Nano Letters*, **16**, 4447 (2016).

58. Huake Liu, Guangzhao Qin, Yuan Lin, and Ming Hu,* "Disparate Strain Dependent Thermal Conductivity of Two-dimensional Penta-Structures", *Nano Letters*, **16**, 3831 (2016).

57. Tao Ouyang,* Huaping Xiao, Chao Tang, Ming Hu,* and Jianxin Zhong, "Anisotropic Thermal Transport in Weyl Semimetal TaAs: a First-principles Calculation", *Physical Chemistry Chemical Physics*, **18**, 16709 (2016).

56. Eungkyu Lee, Teng Zhang, Ming Hu, and Tengfei Luo,* "Thermal Boundary Conductance Enhancement using Experimentally Achievable Nanostructured Interfaces - Analytical Study Combined with Molecular Dynamics Simulation", *Physical Chemistry Chemical Physics*, **18**, 16794 (2016).

55. Yanguang Zhou, Yagang Yao, and Ming Hu,* "Boundary Scattering Effect on Thermal Conductivity of Nanowires", *Semiconductor Science and Technology*, **31**, 074004 (2016).

54. Yang Han, Guangzhao Qin, Christoph Jungemann,* and Ming Hu,* "Strain Modulated Electronic and Thermal Transport Properties of Two-dimensional O-silica", *Nanotechnology*, **27**, 265706 (2016).

53. Guangzhao Qin, Zhenzhen Qin, Wu-Zhang Fang, Li-Chuan Zhang, Sheng-Ying Yue, Qing-Bo Yan,* Ming Hu,* and Gang Su,* "Diverse Anisotropy of Phonon Transport in Two-dimensional Group IV-VI Compounds: A Comparative Study", *Nanoscale*, **8**, 11306 (2016).

52. Yanguang Zhou, Yuli Chen, and Ming Hu,* "Strong Surface Orientation Dependent Thermal Transport in Si Nanowires", *Scientific Reports*, **6**, 24903 (2016).

51. Xiaoliang Zhang, Yufei Gao, Yuli Chen, and Ming Hu,* "Robustly Engineering Thermal Conductivity of Bilayer Graphene by Interlayer Bonding", *Scientific Reports*, **6**, 22011 (2016).

50. Han Xie, Tao Ouyang, Éric Germaneau, Guangzhao Qin, Ming Hu,* and Hua Bao,* "Large Tunability of Lattice Thermal Conductivity of Monolayer Silicene via Mechanical Strain", *Physical Review B*, **93**, 075404 (2016).

49. Yanguang Zhou, Xiaoliang Zhang, and Ming Hu,* "Excellent Candidate for Largely Reducing Interfacial Thermal Resistance: Nano-confined Mass Graded Interface", *Nanoscale*, **8**, 1994 (2016).

48. Tao Ouyang and Ming Hu,* "Competing Mechanism Driving Diverse Pressure Dependence of Thermal Conductivity of XTe (X = Hg, Cd, and Zn)", *Physical Review*

B, **92**, 235204 (2015).

47. Yanguang Zhou and Ming Hu,* “Quantitatively Analyzing Phonon Spectral Contribution of Thermal Conductivity Based on Non-Equilibrium Molecular Dynamics Simulation II: From Time Fourier Transform”, *Physical Review B*, **92**, 195205 (2015).

46. Yanguang Zhou, Xiaoliang Zhang, and Ming Hu,* “Quantitatively Analyzing Phonon Spectral Contribution of Thermal Conductivity Based on Non-Equilibrium Molecular Dynamics Simulation I: From Space Fourier Transform”, *Physical Review B*, **92**, 195204 (2015).

45. Yang Han and Ming Hu,* “Ground State of Bilayer α -silica: Mechanical and Electronic Properties”, *Nanotechnology*, **26**, 505702 (2015).

44. Yanguang Zhou,* Weiwei Wang, and Ming Hu, “The typical manners of dynamic crack propagation along the metal/ceramics interfaces: A molecular dynamics study”, *Computational Materials Science*, **112**, 27 (2016).

43. Sheng-Ying Yue, Tao Ouyang, and Ming Hu,* “Diameter Dependence of Lattice Thermal Conductivity of Single-Walled Carbon Nanotubes: Study from Ab Initio”, *Scientific Reports*, **5**, 15440 (2015).

42. Yingyan Zhang,* Qing-Xiang Pei, Ming Hu, and Zhi Zong, “Thermal Conductivity of Oxidized Gamma-Graphyne”, *RSC Advances*, **5**, 65221 (2015).

41. Tao Ouyang and Ming Hu,* “First-principles Study on Lattice Thermal Conductivity of Thermoelectrics HgTe in Different Phases”, *Journal of Applied Physics*, **117**, 245101 (2015).

40. Ming Hu,* Yuhang Jing, and Xiaoliang Zhang, “Low Thermal Conductivity of Graphyne Nanotubes from Molecular Dynamics Study”, *Physical Review B*, **91**, 155408 (2015).

39. Yufei Gao, Xiaoliang Zhang, Yuhang Jing, and Ming Hu,* “The Unexpected Non-monotonic Inter-layer Bonding Dependence of the Thermal Conductivity of Bilayered Boron Nitride”, *Nanoscale*, **7**, 7143 (2015).

38. Matthew C. Wingert, Soonshin Kwon, Ming Hu, Dimos Poulidakos,* Jie Xiang,* and Renkun Chen,* “Sub-Amorphous Thermal Conductivity in Ultra-Thin Crystalline Silicon Nanotubes”, *Nano Letters*, **15**, 2605 (2015).

37. Xiaoliang Zhang, Hua Bao,* and Ming Hu,* “Bilateral Substrate Effect on the Thermal Conductivity of Two-dimensional Silicon”, *Nanoscale*, **7**, 6014 (2015).

36. Yuhang Jing, Ming Hu,* Yufei Gao, Licheng Guo, and Yi Sun, “On the Origin of Abnormal Phonon Transport of Graphyne”, *International Journal of Heat and Mass Transfer*, **85**, 880 (2015).

35. Guangzhao Qin, Qing-Bo Yan,* Zhenzhen Qin, Sheng-Ying Yue, Ming Hu,* and Gang Su,* “Anisotropic Intrinsic Lattice Thermal Conductivity of Phosphorene from First Principles”, *Physical Chemistry Chemical Physics*, **17**, 4854 (2015).

34. Tao Ouyang, Xiaoliang Zhang, and Ming Hu,* “Thermal Conductivity of Ordered-Disordered Material: a Case Study of Superionic Ag_2Te ”, *Nanotechnology*, **26**, 025702 (2015).

33. Yanguang Zhou, Yuli Chen,* Bin Liu, Shengtao Wang, Zhenyu Yang, and Ming Hu, “Mechanics of Nanoscale Wrinkling of Graphene on a Non-developable Surface”,

Carbon, **84**, 263 (2015).

32. Tao Ouyang and Ming Hu,* “Thermal Transport and Thermoelectric Properties of Beta-Graphyne Nanostructures”, *Nanotechnology*, **25**, 245401 (2014).
31. Han Xie, Ming Hu,* and Hua Bao,* “Thermal Conductivity of Silicene from First-principles”, *Applied Physics Letters*, **104**, 131906 (2014).
30. Xiaoliang Zhang, Han Xie, Ming Hu,* Hua Bao,* Shengying Yue, Guangzhao Qin, and Gang Su, “Thermal Conductivity of Silicene Calculated Using an Optimized Stillinger-Weber Potential”, *Physical Review B*, **89**, 054310 (2014).
29. Hua Bao,* Cheng Shao, Shirui Luo, and Ming Hu,* “Enhancement of Interfacial Thermal Transport by Carbon Nanotube-Graphene Junction”, *Journal of Applied Physics*, **115**, 053524 (2014).
28. Yuhang Jing and Ming Hu,* “Phonon Transport of Rough Si/Ge Superlattice Nanotubes”, *Computers, Materials, & Continua*, **38**, 43 (2013).
27. Yuhang Jing, Ming Hu,* and Licheng Guo, “Thermal Conductivity of Hybrid Graphene/Silicon Heterostructures”, *Journal of Applied Physics*, **114**, 153518 (2013).
26. Ming Hu,* Xiaoliang Zhang, and Dimos Poulikakos, “Anomalous Thermal Response of Silicene to Uniaxial Stretching”, *Physical Review B*, **87**, 195417 (2013).
25. Xiaoliang Zhang, Ming Hu, and Dawei Tang,* “Thermal Rectification at Silicon/Horizontally Aligned Carbon Nanotube Interfaces”, *Journal of Applied Physics*, **113**, 194307 (2013).
24. Ming Hu and Dimos Poulikakos,* “Graphene Mediated Thermal Resistance Reduction at Strongly Coupled Interfaces”, *International Journal of Heat Mass Transfer*, **62**, 205 (2013).
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22. Xiaoliang Zhang, Ming Hu,* and Dimos Poulikakos, “A Low Frequency Wave Motion Mechanism Enables Efficient Energy Transport in Carbon Nanotubes at High Heat Fluxes”, *Nano Letters*, **12**, 3410 (2012).
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- **Invited talks and presentations**

15. Workshop on “Recent Progress in the Physics of Thermal Transport”, Izmir, Turkey, “Thermal Transport in Advanced Energy Systems - An Interdisciplinary Study of Phonons beyond Lattice Vibration”, 07.2017

14. Keynote speaker at “International Conference on Computational & Experimental Engineering and Sciences” (ICCES’13), Funchal, Madeira, Portugal, “Thermal Transport in Advanced Energy Systems - An Interdisciplinary Study of Phonons beyond Lattice Vibration”, 06.2017

13. EMN Meeting on Nanowires, Amsterdam, Netherlands, “Engineering Phonon Transport in Silicon Nanowires for Advanced Energy Conversion”, 05.2016

12. EMN Meeting on Thermoelectric Materials, Orlando, FL, USA, “First-principles Assisted Novel Thermoelectric Materials Exploration: Challenges and New Strategies”, 02.2016

11. Workshop on Thermal Nanosciences and Nanoengineering, Paris, France, “Strained Phonons from First-principles Study”, 11.2015

10. CECAM Workshop “Hot Nanostructures: heat transport at the nanoscale”, Mainz, Germany, “Strain Effect on the Lattice Thermal Conductivity of 2D and 3D Materials”, 09.2015

9. Institute of Solid Mechanics, Beihang University, Beijing, China, “Mechanical Deformation and Phonons”, 08.2015

8. Department of Engineering Mechanics, Tsinghua University, Beijing, China, “First Principles Study of Strained Phonons”, 08.2015

7. School of Materials and Metallurgy, Northeastern University, Shenyang, China, “Computer Simulation of Nano-Scale Heat Transfer”, 08.2015

6. Department of Physics, Liege University, Belgium, “Phonon Transport in Low-dimensional Silicon-based Structures”, 06.2014

5. Suzhou Institute of Nano-Tech and Nano-Bionics, Chinese Academy of Sciences, Suzhou, China, “Computational Modeling of Nanostructured Materials for Improved Thermal Management”, 03.2014

4. State Key Lab of High Performance Ceramics and Superfine Microstructure, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Suzhou, China, “Nanoscale Phonon Transport with Application in Thermoelectrics”, 03.2014

3. State Key Lab of Non-linear Mechanics, Institute of Mechanics, Chinese Academy of Sciences, Beijing, China, “Nanoscale Heat Transfer in Novel Energy Application”, 12.2013

2. Lehrstuhl und Institut für Eisenhüttenkunde (IEHK), RWTH Aachen University, Aachen, Germany, “Nanomaterials: Meet Challenges in Novel Energy Application”, 10.2013

1. International Conference on Computational & Experimental Engineering and Sciences” (ICCES’13), Seattle, US, “Computational Modeling of Nanostructured Materials for Novel Energy Application”, 05.2013