

Hasan Babaei

Department of Chemical and Petroleum Engineering, University of Pittsburgh
Department of Mechanical Engineering, Carnegie Mellon University

- EXPERIENCE**
- Post-Doctoral Associate** **Sep 2014-Present**
Department of Chemical and Petroleum Engineering, University of Pittsburgh
Department of Mechanical Engineering, Carnegie Mellon University (CMU)
Project Title: *Thermal transport in Metal Organic Frameworks (MOFs)*
Supervisors: Professor C. Wilmer and Professor A. McGaughey
- Visiting Scholar** **Aug 2013-Aug 2014**
Department of Mechanical Engineering, University of Illinois at Urbana-Champaign (UIUC)
Project Title: *Thermoelectric properties of single layer MoS₂ by using ab initio calculations*
Supervisor: Professor S. Sinha
- EDUCATION**
- PhD in Mechanical Engineering,** **Aug 2009-Aug 2014**
Department of Mechanical Engineering, Auburn University **GPA : 4.0/4.0**
Thesis Title: *Molecular-Level Modeling of Thermal Transport Mechanisms within Carbon Nanotube/Graphene-based Nanostructure-Enhanced Phase Change Materials*
Advisors: Professor J. M. Khodadadi and Professor P. Keblinski, RPI
- MS in Mechanical Engineering,** **Sep 2006- June 2009**
Department of Mechanical Engineering, University of Tehran, Tehran, Iran, **GPA: 18.24/20**
Thesis Title: *Simulation of Turbulent Vortex Shedding Past a Square Cylinder near a Wall*
Advisor: Professor M. Raisee
- BS in Mechanical Engineering,** **Sep 2002- July 2006**
Department of Mechanical Engineering, Iran University of Science & Technology **GPA: 17.28/20**
Thesis Title: *Analysis of Turbulent Flow through a Channel using 2nd and 3rd Grade Fluids*
Advisor: Professor Gh. Atefi
- RESEARCH INTERESTS**
- Energy storage and conversion, Nanoscale transport, Nanostructured materials, Colloidal suspensions, Interface, Phase change, Nano-porous materials.
- AWARDS AND HONORS**
- Auburn University *Distinguished Dissertation Award* (Only 3 students awarded in 2016)
 - AU Samuel Ginn CoE Fellowship, Auburn University (2009)
 - AL-EPSCoR GRSP Fellowship (three years, 2010-2011, 2012-2013 and 2013-2014)
 - Ranked among Top 5% of Students (M. Sc., University of Tehran, Tehran, Iran, 2008)
 - Ranked among Top 5% of Students (B. Sc., Iran University of Science and Technology, Tehran, Iran, 2006)
 - Ranked 90th in the M. Sc. Entrance Exam in Mechanical Engineering among more than 11,000 Participants (2006)
 - Ranked 430th in the Nationwide University Entrance Examination among more than 400,000 participants (2002).
 - 2014 Science and Technology Open House Poster Winner (Feb 2014, Montgomery, AL)
 - Auburn Graduate Travel Award

RESEARCH PROJECTS

- Thermal transport in Metal Organic Frameworks (MOFs)
- Biogas purification using MOFs
- MOF arrays for gas sensors
- Ab initio calculations of phonon relaxation times in single layer MoS₂ (Aug 2013-Aug 2014)
- Effect of Nanoparticles on Thin Film Lubrication (Dec 2012-Dec 2013)
- Aggregation of graphene nanosheets in paraffin mixtures upon freezing (July 2012-Mar 2013)
- Determination of interfacial thermal resistance between graphene and solid/liquid paraffin by using Molecular Dynamics (Apr 2011-2013)
- Paraffin crystalline structure-thermal transport relationship with emphasis on effect of carbon nanotube and graphene by using atomistic simulation (Sep 2011-June 2012)
- Heat transfer mechanisms in nanofluids by utilizing molecular dynamics simulations (Aug 2010-Aug 2013)
- Force field parameterization for water using Quantum Calculations (Sep 2010-May 2011)
- Non-Continuum Modeling of NePCM (Aug 2009 –Aug 2013)
- Simulation of Turbulent Vortex Shedding Past a Square Cylinder Near a Wall (Sep 2006 –June 2009)
- Analysis of Turbulent Flow through a Channel using 2nd and 3rd Grade Fluids (July 2004 – Sep 2006)

JOURNAL PUBLICATIONS

- 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 (2016).
- H. Babaei** and C. E. Wilmer, *Mechanisms of Heat Transfer in Porous Crystals Containing Adsorbed Gases: Applications to Metal-Organic Frameworks*, Physical Review Letters **116**, 025902 (2016). **PRL Editors' Suggestion.**
- H. Babaei**, J. M. Khodadadi, and S. Sinha, *Large theoretical thermoelectric power factor of suspended single-layer MoS₂*, Applied Physics Letter **105**, 193901 (2014).
- R. L. Jackson, H. Ghaednia, **H. Babaei**, J. M. Khodadadi, *Comment on Šperka, P., I. Křupka, M. Hartl (2014). "Evidence of Plug Flow in Rolling–Sliding Elastohydrodynamic Contact."*, Tribology Letters **54** (2), 151–160 (2014).
- H. Ghaednia, **H. Babaei**, R. L. Jackson, M. J. Bozack, J. M. Khodadadi, *The effect of nanoparticles on thin film elasto-hydrodynamic lubrication*, Applied Physics Letters, **103**(26), 263111 (2013). ***The first two authors contributed equally to this work*.**
- H. Babaei**, P. Keblinski, and J. M. Khodadadi, *Improvement in thermal conductivity of paraffin by adding high aspect-ratio carbon-based nano-fillers*, Physics Letters A, **377**, 1358–1361 (2013).
- H. Babaei**, P. Keblinski, and J. M. Khodadadi, *A Proof for Insignificant Effect of Brownian Motion-Induced Micro-Convection on Thermal Conductivity of Nanofluids by Utilizing Molecular Dynamics Simulations*, J. Appl. Phys, **113**, 084302 (2013).
- J. M. Khodadadi, Liwu Fan and **Hasan Babaei**, *Thermal Conductivity Enhancement of Nanostructure-Based Colloidal Suspensions Utilized as Phase Change Materials for Thermal Energy Storage: A Review*, Renewable & Sustainable Energy Reviews, **24**, 418 (2013).
- H. Babaei**, P. Keblinski, and J. M. Khodadadi, *Thermal conductivity enhancement of paraffin by increasing the alignment of molecules through adding CNT/Graphene*, International Journal of Heat and Mass Transfer, **58**, 209 (2013).
- H. Babaei**, P. Keblinski, and J. M. Khodadadi, *Equilibrium Molecular Dynamics Determination of Thermal Conductivity for Multi-Component Systems*, J. Appl. Phys. **112**, 054310 (2012).
- M. Raisee, A. Jafari, **H. Babaei**, H. Iacovides, *Two-Dimensional Prediction of Time-Dependent, Turbulent Flow around a Square Cylinder Confined in a Channel*, International Journal for Numerical Methods in Fluids, **62**, 1232 (2010).

**PAPERS TO BE
SUBMITTED OR
UNDER
PROGRESS**

- H. Babaei**, A. J. H. McGaughey and C. E. Wilmer, *Transient molecular simulation of gas adsorption into metal-organic frameworks: heat and mass transfer phenomena*, to be submitted.
- H. Babaei**, A. J. H. McGaughey and C. E. Wilmer, *Heat Transfer in Porous Crystals*, under progress.
- H. Babaei**, J. M. Khodadadi, and S. Sinha, *Phonon relaxation times for single-layer MoS₂ from ab initio calculations*, under progress.
- H. Babaei**, M. Raisee, *Modeling of Vortex Shedding Turbulent Flow around a Square Cylinder near a Wall*, to be submitted to International Journal for Numerical Methods in Fluids.

**CONFERENCE
PUBLICATIONS**

- H. Babaei**, Christopher E. Wilmer, *Heat Transfer in Porous Crystals Containing Adsorbed Gases*, Bulletin of the American Physical Society 2016.
- H. Babaei**, J. M. Khodadadi, and Sanjiv Sinha, *Relaxation Times of Single-Layer MoS₂*, MRS Spring 2015.
- Krishna V. Valavala, **H. Babaei**, and Sanjiv Sinha, *Thermoelectric Power Factor Measurement on Monolayer MoS₂*, MRS Spring 2015.
- H. Babaei**, Christopher E. Wilmer, *Heat Transfer Mechanisms in Metal-Organic Frameworks during Natural Gas Storage Adsorption*, MRS Spring 2015.
- H. Babaei**, J. M. Khodadadi, and Sanjiv Sinha, *Phonon Relaxation Times and Thermoelectric Properties of Single-Layer MoS₂*, MRS Spring 2014.
- H. Babaei**, P. Keblinski, and J. M. Khodadadi, *Molecular dynamics study of the interfacial thermal conductance at the graphene/paraffin interface in solid and liquid phases*, ASME HT2013.
- H. Ghaednia, **H. Babaei**, R.L. Jackson, M. J. Bozack, J. M. Khodadadi, “The Effect of Nanoparticle Additives in the Elasto-hydrodynamic Lubrication Regime”, 68th Annual Meeting and Exhibition of the Society of Tribologists and Lubrication Engineers (STLE 2013), 5-9 May, Detroit, MI.
- H. Babaei**, *Thermal conductivity enhancement of paraffins by increasing the alignment of molecules through adding CNT/Graphene*, LAMMPS workshop, Aug 6-8, 2013.
- H. Ghaednia, **H. Babaei**, R.L. Jackson, M. J. Bozack, J. M. Khodadadi, “The Effect of Nanoparticle Additives in the Elasto-hydrodynamic Lubrication Regime”, Tribology and Lubrication Technology (TLT), Dec 2013, STLE.
- H. Babaei**, P. Keblinski, and J. M. Khodadadi, *Thermal conductivity enhancement of paraffin by increasing the alignment of molecules through adding CNT/Graphene*, 49th Annual Technical Meeting of the Society of Engineering Science, Oct. 12-14, 2012.
- H. Babaei**, *Prediction of Thermal Conductivity of Colloidal Suspensions via Molecular Dynamics Simulations*, LAMMPS workshop, Aug 9-11, 2011.
- H. Babaei**, J. M. Khodadadi, *Prediction of Thermal Conductivity of a Model Nanofluid via Molecular Dynamics Simulations*, Thermal and Materials Nanoscience and Nanotechnology, Antalya, Turkey, May 29 – June 3, 2011.
- H. Babaei**, J. M. Khodadadi, *Prediction of Thermal Conductivity of Liquid Methane/Ethane-Cu Nanofluids via Molecular Dynamics Simulations*, TechConnect World Conference and Trade Show, June 13-16, 2011, Boston, Massachusetts, U.S.A.
- H. Babaei**, M. Raisee, *Simulation of Turbulent Flow around a Square Cylinder Near a Wall*, 12th Annual Int. Conf. Fluid Dynamics, Iran, 2008.
- H. Babaei**, M. Raisee, *Modeling of Vortex Shedding Turbulent Flow around a Square Cylinder near a Wall*, Turbulence, Heat and Mass Transfer Conference, Italy, 2009.
- H. Babaei**, Gh. Atefi, *Analysis of Turbulent Flow through a Channel using 2nd and 3rd Grade Fluids*, 14th Annual Int. Conf. on Mech. Eng., Isfahan University of Technology, Iran, May 2006.

**FUNDED PEER-
REVIEWED
PROPOSALS**

- ACS Petroleum Research Fund, 2015-2018 (\$110,000, PI: Chris E. Wilmer)
- AL-EPSCoR GRSP Fellowship 2010-2011 (\$25,000)
- AL-EPSCoR GRSP Fellowship 2012-2013 (\$25,000)
- AL-EPSCoR GRSP Fellowship 2013-2014 (\$25,000)

IN NEWS	United Press International , phys.org , Science Codex , EurekAlert , NGT News , Tribune Review , ScienceDaily ,
SELECTED COURSES	Scientific Visualization (audited, Pitt), Molecular Modelling (audited, CMU), Computational Materials Science and Engineering (audited, UIUC MSE), Statistical Mechanics (physics), Advanced Topics in Thermal and Statistical Physics (physics), Intra/Inter-Molecular Forces (chemistry), Theories and Simulations of Thermal Conductivity (physics), Computational Chemistry (audited, chemistry), Molecular Electronic Structure Theory (audited, chemistry), Chemical Kinetics (chemistry), Solid State Physics (audited, physics), Advanced Fluid Mechanics I, Transport Phenomena, Advanced Fluid Mechanics II, Boundary Layer Theory, Continuum Mechanics, Advanced Numerical Methods, Advanced Engineering Mathematics, Advanced Fluid Mechanics, Turbulent Fluid Flow, Advanced Convection Heat Transfer, Advanced Conduction Heat Transfer, Advanced Thermodynamics, Computational Fluid Dynamics
REFREE/ REVIEWER	<ul style="list-style-type: none"> • ACS Nano • ACS Applied Materials and Interfaces (3 manuscripts) • Physical Chemistry Chemical Physics • Carbon (2 manuscripts) • Applied Physics Letters (2 manuscripts) • Journal of Applied Physics (7 manuscripts) • Advanced Materials • International Journal of Heat and Mass Transfer • Journal of Heat Transfer • Composites Science and Technology • Chemical Engineering Science • Solar Energy Materials and Solar Cells • Journal of Renewable and Sustainable Energy • Solar Energy • Materials • Energy Technology • Journal of Computational Electronics • Particuology
TECHNICAL SKILLS	<ul style="list-style-type: none"> • Molecular Dynamics (MD) Simulation • DFT calculation • Quantum Chemistry Simulation • Grand canonical Monte Carlo (GCMC) simulations • Lattice Dynamics • Computational Fluid Dynamics
COMPUTER SKILLS	<ul style="list-style-type: none"> • Operating Systems: Linux, Windows • Programming Languages: Fortran, Python • Software: LAMMPS (MD package), Quantum Espresso (DFT and AIMD package), VASP (DFT and AIMD package), CPMD (Car-Parrinello MD package), RASPA (Molecular package for Adsorption and Diffusion), GULP, Jaguar (Quantum calculations), GROMACS (MD package), VMD, Packmol, Atomeye, Fluent, Gambit, Tecplot, AutoCAD, Mechanical Desktop, Mathematica, MATLAB, Microsoft Office

TEACHING

- Teaching Assistant, University of Tehran, General Mathematics, Fall 2006-Spring 2007

EXPERIENCE

- Teaching Assistant, Auburn University, Fluid Mechanics, Fall 2009-Spring 2010
- Teaching Assistant, Auburn University, Introduction to Thermodynamics, Fluids And Heat Transfer, Fall 2009-Spring 2010

REFERENCES

- Prof. Christopher E. Wilmer, Chemical/Petroleum Engineering, University of Pittsburgh, 3700 O'Hara St. Pittsburgh, PA 15261, USA. Phone: 412-624-9154, Email: wilmer@pitt.edu
- Prof. Jay M. Khodadadi, Mechanical Engineering, Auburn University, 1418 Wiggins Hall, Auburn, Alabama 36849-5341, USA. Phone: 334-844-3333, Email: khodajm@auburn.edu
- Prof. Pawel Koblinski, Materials Science & Engineering, Rensselaer Polytechnic Institute (RPI), Materials Research Center, Troy, New York, 12180. Phone: 518-276-6858, Email: keblip@rpi.edu
- Prof. Sanjiv Sinha, Mechanical Science & Engineering, University of Illinois at Urbana-Champaign (UIUC). Phone: 217-244-1891, Email: sanjiv@illinois.edu
- Prof. Alan McGaughey, Mechanical Engineering, Carnegie Mellon University, 5000 Forbes Avenue, Scaife Hall 414 Pittsburgh, PA 15213, USA. Phone: 412-268-9605, Email: mcgaughey@cmu.edu
- Prof. Rik Blumenthal, Chemistry and Biochemistry, Auburn University. Email: blumeri@auburn.edu