

# Pengfei Ji

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## Professional Summary

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- ◆ Diligent and highly motivated Ph.D. with 9 years experiences in thermal & mechanical engineering.
- ◆ *Ab initio* calculation, molecular dynamics, computational fluid mechanics and heat transfer.
- ◆ Proficient utilization of Python, C, C++ and Fortran in numerical programming & analysis.
- ◆ Excellent software engineer known for developing a multiscale simulation code QMTIS (*Quantum-mechanics Molecular-dynamics Two-temperature-model Integrated Simulator*).

## Educational Background

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<b>Ph.D.</b>	Mechanical Engineering	University of Missouri-Columbia, USA	2013 – 2016
	Advised by Professor Yuwen Zhang (Homepage: <a href="http://mtt.missouri.edu/Zhang.html">http://mtt.missouri.edu/Zhang.html</a> )		
	Dissertation: <i>Multiscale Modeling and Simulation of Laser Interaction with Metals</i>		
<b>M.S.</b>	Mechanical Engineering	University of Missouri-Columbia, USA	2011 – 2013
	Thesis: <i>Ab Initio Molecular Dynamics Study of Nanoscale Heat Transfer &amp; Energy Conversion</i>		
<b>B.S.</b>	Mechanical Engineering	North China Electric Power University, China	2007 – 2011

## Professional Experiences

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### ◆ Scientific Research

#### ● Multiscale Modeling and Simulation

Ultrashort laser material interaction is systematically carried out. A database containing thermophysical parameters from *ab initio* electron structural calculations is constructed. Selective data at given electron temperature are dynamically implemented into the molecular-dynamics and two-temperature-model coupled simulation. Laser heating induced thermal melting, layer-ablation and explosive boiling are observed in the simulation results. Numerical methods, such as polynomial interpolation, linear regression and numerical integration are programmed for the calculation process.

#### ● Nanoscale Heat Transfer

As an ideal thermoelectric material, the nanoscale heat conduction and thermal radiation between Si/Ge superlattices are investigated by utilizing *ab initio* molecular dynamics. The post-processing of atomic trajectories is programmed by using Python and Gnuplot. Lattice structural change, atomic thermal motion and vibrational spectrum are visualized.

#### ● Ultrashort Laser Induced Period Surface Structures

The periodic surface structures is generated by applying ultrashort laser pulses irradiation. Scan electron microscopy (SEM) images are taken to get nanoscale sights into the periodic surface structure. Energy Dispersive Spectroscopy (EDS) is implemented to analyze the elements of laser irradiated surface.

### ◆ Software Development

#### ● A multiscale simulation program: QMTIS <https://github.com/PengfeiJi2htec/QMTIS>

The program has highly modular structure, which is written by C++ and Fortran for parallel computing (OpenMPI library), C, Python and Gnuplot for pre-/post-processing. The two parts of C++ and Fortran programs are hierarchically coupled by using Shell Script. The QMTIS

program is developed and runs with command input file.

- **MTTL (Multiscale Thermal Transport Laboratory)** <http://mtt.missouri.edu>  
The site is designed and programmed by using HTML language. In order to dynamically show the pictures in the homepage, JavaScript is implemented. The website presents comprehensive information that covers scientific research, published papers and updates of progress in MTTL.
- **Cloud System for Experimental Research and Online Teaching**  
A cloud system is established by using [Joomla](#), which enables student make reservation for experimental research, perform online examination, submit homework and exchange their ideas. The functional module is developed by PHP and MySQL.

## Core Skills

Programming language:	Scientific Research:	Software proficiency:	Supercomputer:
<i>Python, C, C++, Fortran, Shell Script, JavaScript, PHP, Gnuplot and HTML.</i>	<i>Multiscale Modeling, First Principles Calculation, CFD.</i>	<i>CPMD, ABINIT, IMD, LAMMPS, OpenFOAM, ANSYS, COMSOL.</i>	<i>High performance computing (HPC) and parallel coding.</i>

## Graduate Courses

Heat Transfer Convection	A	Computational Heat Transfer and Fluid Mechanics	A
Microscale Heat Transfer	A <sup>+</sup>	Advanced Thermodynamics	A
Statistical Mechanics	A	Quantum Chemistry	A
Numerical Linear Algebra	A	Introduction of MEMS	A
Computational Chemistry	A <sup>+</sup>	Thermodynamics and Statistical Mechanics	A <sup>+</sup>

## Research Publications

### ◆ Journal Publications

1. **Ji, P.**, and Zhang, Y., 2013, “[First-Principles Molecular Dynamics Investigation of the Atomic-Scale Energy Transfer: From Heat Conduction to Thermal Radiation](#)”, *International Journal of Heat and Mass Transfer*, 60, 69-80.
2. **Ji, P.**, Zhang, Y., and Yang, M., 2013, “[Femtosecond Laser Processing of Germanium: An Ab Initio Molecular Dynamics Study](#)”, *Journal of Physics D: Applied Physics*, 46, 495108.
3. **Ji, P.**, and Zhang, Y., 2013, “[Structural, Dynamic, and Vibrational Properties during Heat Transfer in Si/Ge Superlattices: A Car-Parrinello Molecular Dynamics Study](#)”, *Journal of Applied Physics*, 114, 234905.
4. **Ji, P.**, and Zhang, Y., 2016, “[Continuum-atomistic Simulation of Picosecond Laser Heating of Copper with Electron Heat Capacity from Ab Initio Calculation](#)”, *Chemical Physics Letters*, 648, 109-113.
5. **Ji, P.**, and Zhang, Y., 2016, “[Ab initio Determination of Effective Electron-phonon Coupling Factor in Copper](#)”, *Physics Letters A*, 380, 1551-1555.
6. **Ji, P.**, and Zhang, Y., 2016, “[Multiscale Modeling of Femtosecond Laser Irradiation on Copper Film with Electron Thermal Conductivity from Ab Initio Calculation](#)”, *Numerical Heat Transfer, Part A*, 71, 128-136.
7. **Ji, P.**, and Zhang, Y., 2017, “[Electron-Phonon Coupled Heat Transfer and the Corresponding Thermal Response Induced by Femtosecond Laser Heating of Gold](#)”, *ASME Journal of Heat Transfer*, 139, 052001.
8. Li, L., **Ji, P.**, and Zhang, Y., 2016, “[Molecular Dynamics Simulation of Condensation on](#)

[Nanostructured Surface in a Confined Space](#)", *Applied Physics A: Materials Science & Processing*, 122, 496.

9. Li, Y., Li, Y., **Ji, P.**, and Yang, J., 2015, "[Development of Energy Storage Industry in China: A Technical and Economic Point of Review](#)", *Renewable and Sustainable Energy Reviews*, 49, 805-812.
10. Li, Y., Li, Y., **Ji, P.**, and Yang, J., 2015, "[The Status Quo Analysis and Policy Suggestions on Promoting China's Hydropower Development](#)", *Renewable and Sustainable Energy Reviews*, 51, 1071-1079.

#### ◆ Conference Proceedings

1. **Ji, P.**, and Zhang, Y., "Ab Initio Molecular Dynamics Study of Structural, Dynamic, and Vibrational Properties of Si/Ge Superlattices during Heat Transfer". *International Mechanical Engineering Congress and Exposition*, San Diego, November 15-21, 2013.
2. **Ji, P.**, and Zhang, Y., "An Ab Initio Molecular Dynamics Simulation of Femtosecond Laser Processing of Germanium". *ASME 2013 4th Micro/Nanoscale Heat & Mass Transfer International Conference*, Hong Kong, China, December 11-14, 2013.
3. Gruzdev, V., **Ji, P.**, Chen, J.K., Cooper, B., and Zhang, Y., "Nanostructuring of Rough Aluminum Surface by Ultrashort Laser Pulses: Influence of Laser Fluence," *Conference on Lasers and Electro-Optics (CLEO)*, San Jose, CA, May 10-15, 2015.
4. Afrin, N., **Ji, P.**, Zhang, Y., and Chen, J.K., "Effects of Beam Size and Pulse Duration on the Laser Drilling Process," *ASME 2016 Summer Heat Transfer Conference*, Washington, DC, July 10-14, 2016.
5. **Ji, P.**, and Zhang, Y., "Effects of Film Thickness on Femtosecond Laser Spallation and Ablation of Silver Film," *The 2nd Thermal and Fluids Engineering Conference and 4th International Workshop on Heat Transfer*, Las Vegas, NV, USA, April 2-5, 2017.

### **Proposal Writing Experience**

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1. **National Science Foundation (United States)**  
"Ab initio Based Multiscale Modeling of Thermal Transport in Femtosecond Laser Materials Processing"; Funded; Principle Investigator: Yuwen Zhang; From 08-2013 to 08-2016; Award Amount: \$299,995.
2. **National Science Foundation (United States)**  
"Multiscale Dynamics Simulation of Self-Assembly and Transport in Nanoparticulate Systems"; Funded; Principle Investigator: Yuwen Zhang; From 08-2014 to 07-2017; Award Amount: \$364,796.
3. **National Science Foundation (China)**  
"Impacts on the Vulnerability of the Smart Grid Induced by Large-scale Consumption and Acceptance of the Intermittent Electric Power"; Funded; Principle Investigator: Yanbin Li; From 01-2015 to 12-2018; Award Amount: ¥ 620,000.

### **Scholarships & Awards**

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#### ◆ Scholarships

1. Research Assistantship in University of Missouri-Columbia.
2. Excellent Undergraduate of Beijing.
3. Presidential Scholarship in North China Electric Power University (NCEPU).

### ◆ **Competition Awards**

1. National Undergraduates Innovative Project in China.
2. Energy Saving Competition in NCEPU.
3. Power Technology Cup: Students' Business Plan Competition in NCEPU.