

# Linyuan Shi

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## Working Experience

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### Zhengzhou University

Lecturer of School of Materials Science and Engineering

Zhengzhou, China

Aug 2021–Present

## Education

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### University of Florida

Doctor of Philosophy in Material Science and Engineering, Cumulative GPA:3.86

Gainesville, FL

Aug 2016–May 2021

### Central South University

Bachelor of Science in Powder Material Science and Engineering, GPA:88.20/100 Rank:5/88 Sep 2012–Jun 2016

ChangSha, CHINA

## Research Experience

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### Mesoscale Framework for multi-physics simulation of ablative thermal protection system Gainesville, FL

Ph.D. Candidate, Dr. Simon R Phillipot Research Group

Jan 2018–Present

Objective: Develop a multiphysics tool to predict the structure on pyrolysis and ablation of phenolic impregnated carbon ablator(PICA) thermal protection system(TPS).

- o Characterize the structure of carbon fiber and generate the high fidelity carbon fiber model at atomic scale.
- o Measure the mechanical and thermal properties of carbon fiber including tensile strength, thermal conductivity etc.
- o Simulate the pyrolysis and oxidation of carbon fiber under high temperature using accelerated reactive molecular dynamics.

### Mechanical Properties of Zr-H system

Graduate Research Assistant, Dr. Simon R Phillipot Research Group

Gainesville, FL

Feb 2017–Mar 2020

Objective: Investigate the mechanical properties of Zr with H interstitial and ZrH<sub>x</sub> inclusions using nanoindentation.

- o Verify the fidelity of COMB3 potential for ZrH<sub>x</sub> system.
- o Compute mechanical properties of ZrH<sub>x</sub>
- o Analyze load vs. indentation depth, hardness vs. indentation curve of ZrH<sub>x</sub> and investigate deformation mechanisms.

### Molecular dynamics simulation of radiation damage on tungsten

Research assistant, State Key Laboratory of Powder Metallurgy

ChangSha, CHINA

Nov 2015–Jun 2016

Objective: Investigate the mechanical properties, crystal structure stability, thermodynamic performance and stimulate the cascade progress on tungsten.

- o Studied the number and distribution of defects produced by displacement cascades.
- o Analyzed relations between primary knock on atom(PKA) energy and the number of defects at stable state.
- o Found the threshold energy of tungsten at different crystal orientations.

### Evaluation of W–TiC interface cohesion

Research assistant, State Key Laboratory of Powder Metallurgy

ChangSha, CHINA

Nov 2014–Mar 2015

Objective: Reveal the fundamental mechanism in terms of electronic structures and provide a deep understanding to various interface properties of W–TiC.

- o Optimized the bulk lattice constant and crystal structures of W and TiC.
- o Found a proper number of surface layers with a vacuum layer.
- o Calculated the work of separation ( $W_{sep}$ ) of W–TiC interfaces.

## Skills

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### Programming Languages

- o *C/C++*: Familiar with Modern C++ and experienced in C++ STL, smart pointer and templates.
- o *Python*: Skilled in Numpy, Scipy, Pandas and Matplotlib.
- o *Matlab*: Proficient in writing scientific scripts and implementing scientific algorithms.
- o *Fortran*: Implementing and amending scientific algorithms.

### Specialty Software

- o *VASP*: Skillful in computing mechanical and thermodynamics properties of materials and plotting band structures.
- o *LAMMPS*: Familiar with modeling a dynamic process and calculating basic properties of materials.
- o *OVITO*: Experienced with analyzing materials by developing customized plugin via Python interface.
- o *VESTA*: Experienced with visualizing crystal structures and exporting specific format files.

## Honors and Awards

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- ICME summer school fellowship awarded by National Science Foundation, June 2017
- NBTM Outstanding Student Fellowship awarded by NBTM New Material Group Co., Ltd, Fall 2015

## Publication

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- **Linyuan Shi**, Marina Sessim, Michael R. Tonks, and Simon R. Phillpot. "High-temperature oxidation of carbon fiber and char by molecular dynamics simulation." *Carbon* (2021), 185, 449-463
- **Linyuan Shi**, Marina Sessim, Michael R. Tonks, and Simon R. Phillpot. "Generation and characterization of an improved carbon fiber model by molecular dynamics." *Carbon* (2021), 173, 232-244.
- **Linyuan Shi**, Michele L. Fullarton, and Simon R. Phillpot. "Nanoindentation of ZrH<sub>2</sub> by molecular dynamics simulation." *Journal of Nuclear Materials* (2020): 152391.
- **Linyuan Shi**, Marina Sessim, Michael Tonks and Simon Phillpot, Modeling Carbon fiber oxidation under high temperature by ReaxFF based molecular dynamics simulation, "AIAA SciTech Forum, American Institute of Aeronautics and Astronautics, 2020, Chaps."
- Phillpot, Simon R., Andrew C. Antony, **Linyuan Shi**, Michele L. Fullarton, Tao Liang, Susan B. Sinnott, Yongfeng Zhang, and S. Bulent Biner. "Charge Optimized Many Body (COMB) potentials for simulation of nuclear fuel and clad." *Computational Materials Science* 148 (2018): 231-241.
- D.Y. Dang, **L.Y. Shi**, J.L. Fan, H.R. Gong, First-principles study of W-TiC interface cohesion, *Surface and Coatings Technology*, 25 August 2015, ISSN 0257-8972