



Dr. Tao Fan

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➤ EDUCATION

PhD in Materials Science and Engineering Nov. 2018 – Sept. 2022
Skolkovo Institute of Science and Technology Moscow, Russia
Thesis: First-Principles Study of Advanced Thermoelectric Materials: Methodology and Application
Supervisor: Artem R. Oganov

Master in Materials Science Sept. 2015 – Apr. 2018
Northwestern Polytechnical University (985&211) Xi'an, China
Thesis: Study on Thermoelectric Performance of the Mg-Si-Pb Solid Solution
Supervisor: Laifei Cheng, Qingfeng Zeng

Bachelor of Engineering in Composite Materials Sept. 2011 – Jul. 2015
Northwestern Polytechnical University (985&211) Xi'an, China
Thesis: Crystal Structure Prediction and Properties Calculation of Hafnium Nitrides Ceramic
Supervisor: Qingfeng Zeng

➤ RESEARCH EXPERIENCE

Interests: Computational Materials Science, Materials Informatics, Thermoelectric Materials.

Research Intern Nov. 2018 – Sept. 2022
Materials Discovery Laboratory, Skolkovo Institute of Science and Technology

- Developed computational tools for transport properties, including thermal conductivity and electrical conductivity.
- Searched for novel high-performance thermoelectric materials, and found dozens of thermoelectric compounds.

Research Assistant Sept. 2015 – Apr. 2018
International Center for Materials Discovery, Northwestern Polytechnical University

- Managed the computer cluster in the laboratory.
- Participated in the development of software USPEX, mainly focus on building a binary compounds database based on MySQL.
- Developed computational tools for calculating thermoelectric properties, and investigated thermoelectric performance of Mg₂Si-Mg₂Pb solid solutions.

Research Assistant Feb. 2015 – Jun. 2016
Science and Technology on Thermostructural Composite Materials Laboratory, Northwestern Polytechnical University

- Participated in the “Crystal structure prediction and melting behavior of hafnium-based ultra-high temperature ceramic with variable compositions” project, which was supported by **the Natural Science Foundation of China**.
- Executed crystal structure prediction of hafnium nitrides and first-principles calculation of their thermodynamic and mechanic properties.

➤ HONORS

Scholarship for PhD students of Skoltech, level 4 (the highest), 2021 – 2022 academic year.

2016 **Graduate Students' National Scholarship** (¥20000.00, 7 from 237 students).

2016 Northwestern Polytechnical University Fellowship for Graduate Students, **First Class**.

Northwestern Polytechnical University "**Outstanding Master Student**" in 2016.

2014 Northwestern Polytechnical University Fellowship for Undergraduate Students, **First Class**.

Northwestern Polytechnical University "**Outstanding Undergraduate Student**" in 2014.

The **Champion** in Crossroads Autonomous Navigation Race of the 16th National Robot Championship in 2014.

The Second Prize in RoboCup Simulation Group of 2013 China Robot Contest & RoboCup Open.

The First Prize in the 9th Xi'an High-tech Challenge Cup Shaanxi University Students Extracurricular Academic Work Competition.

➤ PUBLICATIONS

- [1] **Tao Fan**, Artem R. Oganov. "Discovery of high performance thermoelectric chalcogenides through first-principles high-throughput screening." *Journal of Materials Chemistry C* **9.38** (2021): 13226 – 13235.
- [2] **Tao Fan**, Artem R. Oganov. "AICON2: A program for calculating transport properties quickly and accurately." *Computer Physics Communications* **266** (2021): 108027.
- [3] **Tao Fan**, Artem R. Oganov. "AICON: A program for calculating thermal conductivity quickly and accurately." *Computer Physics Communications* **251** (2020): 107074.
- [4] Yaqiong Zhong, Debalaya Sarker, **Tao Fan**, Liangliang Xu, Xie Li, Guang-Zhao Qin, Zhong-Kang Han, and Jiaolin Cui. "Computationally Guided Synthesis of High Performance Thermoelectric Materials: Defect Engineering in AgGaTe₂." *Advanced Electronic Materials* **7.4** (2021): 2001262.
- [5] **Tao Fan**, Congwei Xie, Shiyao Wang, Artem R. Oganov, and Laifei Cheng. "First-principles study of thermoelectric properties of Mg₂Si-Mg₂Pb semiconductor materials." *RSC advances* **8.31** (2018): 17168 – 17175.
- [6] Núñez-Valdez Maribel, Zahed Allahyari, **Tao Fan**, Artem R. Oganov. "Efficient technique for computational design of thermoelectric materials." *Computer Physics Communications* **222** (2018):152 – 157.
- [7] Li Ke, Vladislav A. Blatov, **Tao Fan et al.** "A series of Cd(II) coordination polymers based on flexible bis(triazole) and multicarboxylate ligands: topological diversity, entanglement and properties." *CrystEngComm* **19** (2017): 5797.
- [8] **Tao Fan**, Qing-Feng Zeng, Shu-Yin Yu. "Novel compounds in the hafnium nitride system: first-principles study of their crystal structures and mechanical properties." *Acta Physica Sinica* **65.11**(2016): 118102-1 – 118102-13.

➤ CONFERENCES

Oral Speech, XXIII International Conference on Data Analytics and Management in Data Intensive Domains, Focus Session: "Computational Materials Science", Moscow, Russia, October 26, 2021

Poster, FAIR Data Infrastructure for Materials Genomics, June 3 – 5, 2020, Virtual Meeting

Poster, International Symposium on Advanced Functional and Computational Materials, Shenzhen, China, 2017

Poster, The 35th International Conference and the 1st Asian Conference on Thermoelectrics, Wuhan, China, 2016

➤ SYNERGIC ACTIVITIES

- Developer of the AICON, a python software for calculating electron and phonon transport properties of semiconductors (<https://github.com/Baijianlu/AICON2.git>)
- Co-developer of the USPEX, a software for crystal structure prediction using evolutionary algorithm (<https://uspex-team.org/en>)

➤ SKILLS

Computer Skills: Proficient in C, C++, python, shell programming, familiar with development tools such as Visual Studio, Spyder; Familiar with Linux system and common operations; Know basic SQL syntax rules and can operate MySQL database.