Curriculum Vitae

PROFILE:

A highly motivated Ph.D driven by the desire to elucidate the science questions. Ability: DFT calculations, elastic and inelastic neutron scattering experiments, data analysis (python), and solid electrolyte synthesis. Proficient in a variety of software such as Shiver, Dave, VASP, LAMMPS, QUANTUM ESPRESSO, EPW, GSAS, FullProf, AMSET.

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EDUCATION:

2011~2014 High School Zhaoyuan No.2 High School, Xisong Road, Zhaoyuan City, Yantai City, Shandong Province, China

2014~2018 B.S (Physics) University of Jinan

20 18~2023 Ph.D Institute of High Energy Physics, Chinese Academy of Sciences (CAS)

Ph.D (Condensed Matter Physics) China Spallation Neutron Source (CSNS)

2023~Now Postdoc Materials Science and Technology Division, Physical Science Directorate, Oak Ridge National Laboratory

EXPERIENCE:

2016~2018 National Innovation experiment training for college students at University of Jinan. Study the gas sensors under specific atmosphere. Responsible for the material production, sensor welding and testing.

2018~2019 Basic learning in University of Chinese Academy of Sciences

2019~2023 Using the DFT calculations and neutron scattering experiments to study the crystal structure of Li/Na battery materials.

2020~2023 The electronic/phonon transport properties in thermoelectric materials (semiconductor).

2021~2023 Synthesize and test solid-state electrolyte materials (Cl based), combine DFT/MD and quasi-elastic neutron scattering to study the Li motion.

2023~Now Inelastic neutron scattering experiments (phonon) and data analysis (BES and EFRC project)

PROFESSIONAL SKILLS:

DFT Calculations:

1. **Study the basic Properties of Crystal:**

electron density of states, mechanical properties, electronic band structure, the bonding properties and electron charge densities and electron exchange.

Ab initio molecular dynamics investigate ion motions :

the thermal dynamical stability and temperature induced ions motions, the diffusion pathway and diffusion coefficient of selected ions, mechanical properties, radial distribution function**.**

Phase change :

Investigate pressure induced phase changes and the phase change during the charge or discharge process, bonding or layer distance changes during the charge/discharge process

Effects of Coating and Adsorption :

Estimate the influence of coating on the structure, such as the insert of coating elements in crystals and the layer or bonding changes.

Study adsorption properties of the ions or functional group on the surface, analysis the activity of functional group and the charge exchange

2. **Classical Molecular Dynamics Simulation:**

Investigate the ions motions, diffusion coefficient, and the effect of doping and vacancy.

3. **Studying Transport Properties in Semiconductors**

Electronic transport properties:

Seebeck coefficient, electron conductivity, electronic thermal conductivity, lattice thermal conductivity, phonon scattering.

Investigate the phonon transport properties

lattice thermal conductivity, phonon group velocity, phonon phase space, Gruneisen parameters, phonon relaxation times and phonon dispersion curves in semiconductors.

Electron phonon interaction :

Using the EPW module to calculate the phonon linewidth, electron-phonon scattering, and carrier mobility at specified temperature.

Neutron scattering experiments:

1. **Rietveld refinement of XRD or neutron data**

Performing neutron and XRD experiments, then solve the data to analysis the crystal structures

2. **Solid electrolyte material**

Synthesis and performing neutron experiments to study the structure properties and ion motions in the crystal

3. **Analysis of inelastic neutron scattering data**

Conduct inelastic neutron scattering experiments on single crystal samples to investigate phonon branches and on powder samples to determine the phonon density of states. Additionally, developing python-based programs to align and correct experimental data with theoretical models.

AWARDS AND HONORS:

The second-class award in Shandong Province for the National College Students Mathematical Modeling Contest 2016

Chair of information and management system committee (student) in the University of Jinan, 2016~2017

National College Students Innovation and Entrepreneurship Training Program, 2016~2018

Best student award in Chinese Academy of Sciences 2018~2019

The second-class award in chorus contest at Chinese Academy of Sciences 2018

The silver award in chorus contest at Songshan Lake 2019

Best student award in Chinese Academy of Sciences 2020~2021

Second award of Doctoral Scholarship 2020

Doctoral Scholarship of Dongguan Research Department, Institute of High Energy Physics, Chinese Academy of Sciences 2020

Top student award in Chinese Academy of Sciences 2021~2022

First award of Doctoral Scholarship 2021

Instructor in the national science-popularizing public activity--the Chinese Academy of Sciences Public Science Day 2021

National doctoral Scholarship in China 2022

Best students award in the Application of Machine Learning in Condensed Matter Physics (NSFC) 2022

Director's Scholarship (excellence award) in the Institute of High Energy Physics 2022

Best student award in Chinese Academy of Sciences 2022~2023

Instructor in the national science-popularizing public activity--the Chinese Academy of Sciences Public Science Day 2023

SUPERVISOR:

PhD:

Dr. Fangwei Wang

Deputy Director of China Spallation Neutron Source

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PUBLICATIONS:

1、 S Acoustic phonon softening enhances phonon scattering in Zintl-phase II-I-V compounds, ***Shaofei Wang***, Junrong Zhang*, Fangwei Wang*. Physical Review B 23 (108), 235213, 2023.

2、 Intrinsic Ultralow Lattice Thermal Conductivity in Full-Heusler Compound Ba_2AgSb, ***Shaofei Wang***, Junrong Zhang*, Fangwei Wang*, *Physical Review Applied* 17 (3), 034023, 2022.

3、 Tailoring Interphase Structure to Enable High-Rate, Durable Sodium-Ion Battery Cathode, Na Li^1, ***Shaofei Wang[1]***, Enyue Zhao, Wen Yin, Zhigang Zhang, Kang Wu, Juping Xu, Yoshihiro Kuroiwa, Zhongbo Hu, Fangwei Wang, Jinkui Zhao, Xiaoling Xiao, *Journal of Energy Chemistry* 68, 564-571, 2022.

4、 Theoretical investigation of Ti_2B monolayer as powerful anode material for Li/Na batteries with high storage capacity, ***Shaofei Wang***, Junrong Zhang*, Fangwei Wang*, *Applied Surface Science* 538, 148048, 2021.

5、 Zintl Phase BaAgSb: Low Thermal Conductivity and High-Performance Thermoelectric Material in Ab Initio Calculation, ***Shaofei Wang***, Junrong Zhang*, Fangwei Wang*, *Chinese Physics Letters*, 38 (2021) 046301, 2021.

6、 Ni, Beyond Thermodynamic Tuning, Maintains the Catalytic Activity of V Species in $Ni_3(VO_4)_2$ Doped MgH_2, Jiahe Zang, ***Shaofei Wang***, Rongrun Hu, Han Man, Jichao Zhang, Fei Wang, Dalin Sun*, Yun Song*, Fang Fang, *Journal of Materials Chemistry A* 9 (13), 8341-8349, 2021.

7、 Li-Triggered the Superior Catalytic Activity of V in Li_3VO_4: Enabling Fast and Full Hydrogenation of Mg at Lower Temperature, Jiahe Zang, ***Shaofei Wang***, Fang Wang, Ziyao Long, Fangjie Mo, Yuanhua Xia, Fang Fang, Yun Song*, Dalin Sun*, *Journal of Materials Chemistry A* 8 (30), 14935-14943, 2020.

8、 Oxygen vacancy promising highly reversible phase transition in layered cathodes for sodium-ion batteries, Kezhu Jiang, Shaohua Guo, Wei Kong Pang, Xueping Zhang, Tiancheng Fang, ***Shaofei Wang***, Fangwei Wang, Xiaoyu Zhang, Ping He, Haoshen Zhou, *Nano Research* 14 (11), 4100-4106, 2021.

9、 Confirmation for Ultra-fast surface reconstruction enabled by built-in electric field in heterostructued CoS_2/CuS for efficient oxygen evolution of water electrolysis. Han Man, Jingjing Feng ***Shaofei Wang*** et. al, Cell Reports Physical Science, 2022.

10、 Confining Bulk Molecular O_2 by Inhibiting Charge Transfer on Surface Anions Toward Stable Redox Electrochemistry in Layered Oxide Cathodes. Kang Wu, Peilin Ran, ***Shaofei Wang***, Lunhua He, Wen Yin, Baotian Wang, Fangwei Wang, Jinkui Zhao, Enyue Zhao, Nano Energy 108602, 2023.

11、 Enhancing the Whole Migration Kinetics of Na_+ in the Anode Side for Advanced Ultralow Temperature Sodium‐Ion Hybrid Capacitor. Ruan, Jiafeng and Luo, Sainan and ***Wang, Shaofei*** and Hu, Jiaming and Fang, Fang and Wang, Fei and Chen, Min and Zheng, Shiyou and Sun, Dalin and Song, Yun, Advanced Energy Materials 2301509, 2023.

12、 Advancing bandgap tuning: Novel nitrogen doping in KLaTiO4 with uncompromised crystallinity. JWB Li, ***S Wang***, BJ Kennedy, Journal of Environmental Chemical Engineering 12 (3), 112568, 2024.

13*、 Kohn Anomalies in Iridium. ***Shaofei Wang***, Simon Th´ebaud, Duncan H. Moseley, Michael E.Manley, Parul Raghuvanshi, Lucas Lindsay,∗ and Raphael H Hermann (**Draft**)

14*、 Density of Phonon states in ZrN. ***Shaofei Wang,*** Raphael H Hermann, Michael E.Manley (**Draft**)