SHAOFEI WANG

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PROFESSIONAL EXPERIENCES

Postdoctoral Research Associate, Oak Ridge National Laboratory 2023.12-Now

BES-FWP Neutron scattering studies of hybrid excitations:

Supervisor: Dr. Raphaël Hermann, Senior R&D staff, Neutron &X-ray scattering group

- Inelastic neutron scattering in combination with DFT calculations to study lattice dynamic excitations in RuO_2, OsO_4 and Iridium.
- Inelastic and polarized neutron scattering, neutron powder diffraction to study magnetic structure evolutions and excitations in high entropy oxide $Mg_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2}O$ and $Mg_{0.2}Co_{0.2}Ni_{0.2}Cu_{0.2}Zn_{0.2}O$.
- Spin wave spectrum simulations in high entropy oxide by using Sunny.
- Resonant Ultrasound Spectroscopy experiments study the elasticity of Pt.

BES-EFRC Thermal Energy Transport Under Irradiation:

Supervisor: Dr. Michael E Manley, Senior Researcher, Neutron &X-ray scattering group

- Inelastic neutron/X-ray scattering experiments study the lattice dynamic excitations in Uranium nitride, Zirconium nitride and Zr1.5%-UO_2.

Visiting Research Scientist 2023.7-2023-11

Supervisor: Junrong Zhang, Professor, Institute of High Energy Physics, Chinese Academy of Science

- Ionic transportations from the point of DFT calculations

Graduate Research Assistant: 2019.8-2023.6

Supervisor: Fangwei Wang, Professor, Institute of Physics, Chinese Academy of Science

- Study the ions and thermal transportation by using DFT calculation and molecular dynamics simulations.
- Conducted neutron/X-ray powder diffraction experiments to study the materials structure
- Contribute to the safety operation of China Spallation Neutron Source
- Contributed to the authorship of the book *Scientific Development Strategy – Neutron Science and Technology* (Mandarin edition).

Research Intern: 2021.3-2022.3

Supervisor: Enyue Zhao, Associate professor, Songshan Lake Laboratory

- Synthesis the solid electrolyte material Li_2ZrCl_6 and study the materials structure by X-ray and neutron diffraction.

Undergraduate Research Assistant: 2016.3-2017.8

Supervisor: Minghui Shao, Associate professor, School of Physical Science and Technology, University of Jinan

- Designed and tested materials for potential gas sensor applications, including sensor assembly through welding.

EDUCATION

Ph.D., Condensed matter physics 2018.8-2023.6

Institute of High Energy Physics, Chinese Academy of Sciences.

Advisor: Fangwei Wang

Dissertation Title:

"Investigation of ionic and thermal transport by DFT calculations and neutron scattering experiments"

Attended driving school during the summer vacation. 2018.7-2018.8

B.S., Physics 2014.9-2018.7

University of Jinan, Jinan Shandong, China

Advisor: Yi Jin

TECHNICAL SKILLS:

- **Structure Characterization:** Neutron and X-ray powder diffraction, inelastic neutron scattering, polarized neutron powder scattering
- **Software and programming:** LaTeX, DAVE, Shiver, Mantid, MATLAB, GSAS, Fullprof, VDRIVE, Sunny, Python, Adobe Illustrator, VASP, LAMMPS, QUANTUM ESPRESSO, Phonopy, ShengBTE, VASPkit, RUScal.

WORKSHOP:

CV and Résumé Workshop 2025

Advanced Neutron Powder Diffraction Analysis with TOPAS, Oak Ridge, TN 2024

Magnetic Structure Determination from Neutron Diffraction Data (MagStr), Atlanta, GA 2024

Machine Learning in Condensed Matter Physics (NSFC), Zhenjiang, Jiangsu, China 2022

Fullprof Retvield refinement, Shanghai University, Shanghai, China 2021

Neutron and X-ray scattering school, China Spallation Neutron Source, Dongguan, Guangdong, China 2019

PUBLICATIONS:

- **Shaofei Wang**, Simon Thébaud, Duncan H. Moseley, James R. Torres, Michael E. Manley, Yongqiang Cheng, Songxue Chi, Douglas L. Abernathy, Garrett E. Granroth, Andrei T. Savici, Andrew F May, Parul Raghuvanshi, Lucas Lindsay, and Raphaël H. Hermann. Kohn Anomalies and Phonon Anharmonicity in Iridium. (Under review: Physical Review B)
- **Shaofei Wang**, Mark A. Mathis, Chris A. Marianetti, J. Matthew Mann, David B. Turner, Douglas L. Abernathy, Raphaël H Hermann, Michael E. Manley. Lattice dynamics in polycrystalline ZrN. Physical Review B, 111(18), 184316 2025.
- Parul Rani Raghuvanshi, **Shaofei Wang**, Jana Phillips, Valentino Cooper, Lucas Lindsay, Raphaël Hermann, David Parker, Luke Daemen. Lattice dynamics in sparse molecular crystals: OsO_4 and RuO_4. The Journal of Physical Chemistry, 129(15) 2025.
- Parul Rani Raghuvanshi, Tom Berlijn, David Parker, **Shaofei Wang**, Michael Manley, Raphaël Hermann, Lucas Lindsay, Valentino Cooper. Altermagnetic behavior in OsO_2: Parallels with RuO_2. Physical Review Materials, 9(3), 034407 2025.
- JWB Li, **Shaofei Wang**, BJ Kennedy. Advancing bandgap tuning: Novel nitrogen doping in $KLaTiO_4$ with uncompromised crystallinity. Journal of Environmental Chemical Engineering 12 (3), 112568, 2024.
- **Shaofei Wang**, Junrong Zhang, Fangwei Wang. Acoustic phonon softening enhances phonon scattering in Zintl-phase II-I-V compounds. Physical Review B 23 (108), 235213 2023.
- Kang Wu, Peilin Ran, **Shaofei Wang**, Lunhua He, Wen Yin, Baotian Wang, Fangwei Wang, Jinkui Zhao, Enyue Zhao. Confining Bulk Molecular O_2 by Inhibiting Charge Transfer on Surface Anions Toward Stable Redox Electrochemistry in Layered Oxide Cathodes. Nano Energy 108602, 2023.
- Jiafeng Ruan, Sainan Luo, **Shaofei Wang,** Jiaming Hu, Fang Fang, Fei Wang, Min Chen, Shiyou Zheng, Dalin Sun, and Yun Song. Enhancing the Whole Migration Kinetics of Na^+ in the Anode Side for Advanced Ultralow Temperature Sodium-Ion Hybrid Capacitor. Advanced Energy Materials 2301509, 2023.
- **Shaofei Wang**, Junrong Zhang, Fangwei Wang. Intrinsic Ultralow Lattice Thermal Conductivity in Full-Heusler Compound Ba_2AgSb. Physical Review Applied 17 (3), 034023 2022.
- 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. Tailoring Interphase Structure to Enable High-Rate, Durable Sodium-Ion Battery Cathode. Journal of Energy Chemistry 68, 564-571 2022.

- Kezhu Jiang, Shaohua Guo, Wei Kong Pang, Xueping Zhang, Tiancheng Fang, **Shaofei Wang**, Fangwei Wang, Xiaoyu Zhang, Ping He, Haoshen Zhou. Oxygen vacancy promising highly reversible phase transition in layered cathodes for sodium-ion batteries. Nano Research 14 (11), 4100-4106, 2021.
- Han Man, Jingjing Feng, **Shaofei Wang**, Shuyang Li, Peng Li, Huiwen He, Wioletta Raróg-Pilecka, Jie Zhao, Jichao Zhang, Fang Fang, Dalin Sun, Yongtao Li, Yun Song. Confirmation for Ultra-fast surface reconstruction enabled by built-in electric field in heterostructued CoS_2/CuS for efficient oxygen evolution of water electrolysis. Cell Reports Physical Science, 2022.
- **Shaofei Wang**, Junrong Zhang, Fangwei Wang. Theoretical investigation of Ti_2B monolayer as powerful anode material for Li/Na batteries with high storage capacity. Applied Surface Science 538, 148048 2021.
- **Shaofei Wang**, Junrong Zhang, Fangwei Wang. Zintl Phase BaAgSb: Low Thermal Conductivity and High-Performance Thermoelectric Material in Ab Initio Calculation. Chinese Physics Letters 38, 046301 2021.
- Jiahe Zang, **Shaofei Wang**, Rongrun Hu, Han Man, Jichao Zhang, Fei Wang, Dalin Sun, Yun Song, Fang Fang. Ni, Beyond Thermodynamic Tuning, Maintains the Catalytic Activity of V Species in $Ni_3(VO_4)_2$ Doped MgH_2. Journal of Materials Chemistry A 9 (13), 8341-8349 2021.
- Jiahe Zang, **Shaofei Wang**, Fang Wang, Ziyao Long, Fangjie Mo, Yuanhua Xia, Fang Fang, Yun Song, Dalin Sun. Li-Triggered the Superior Catalytic Activity of V in Li_3VO_4: Enabling Fast and Full Hydrogenation of Mg at Lower Temperature. Journal of Materials Chemistry A 8 (30), 14935-14943 2020.

PRESENTATIONS&CONFERENCE:

Poster: Phonon lifetimes in ordered and disordered nuclear materials: Neutron scattering and theory, 2025 EFRC-Hub-CMS-CCS PI Meeting, Rockville, MD, Aug 11-12, 2025.

Oral: Investigation of Phonon Density of States in ZrN and Inelastic Neutron Scattering, 13th annual ORPA research Symposium, Oak Ridge, TN, Jul 17-18, 2025.

Oral: Density of Phonon States in ZrN by neutron scattering and DFT calculations, TMS 154th Annual Meeting &Exhibition, Las Vegas Nevada, Mar 23-27, 2025.

Oral: Kohn Anomalies in Iridium by Neutron scattering and DFT Calculations, APS Global Physics Summit, Anaheim, California, Mar 16-21, 2025.

Oral: Measurements of Density of phonon States in ZrN, EFRC-TETI all hands meeting, Columbus, Ohio, Nov 11-15, 2024.

Poster: Kohn Anomalies in Iridium from Inelastic Neutron Scattering and DFT calculations, American Conference on Neutron Scattering, Knoxville, TN, Jun 23-27, 2024.

Poster: Intrinsic Ultralow Lattice Thermal Conductivity in Full-Heusler Compound Ba_2AgSb. Physical Annual Conference in Guangdong, Chaoshan, Guang Dong, China, Dec 3-6, 2021.

Poster: Theoretical investigation of Ti_2B monolayer as powerful anode material, China Spallation Neutron Source User Annual Meeting and User Committee Meeting, Dongguan, Guangdong, China, Sep 12-13, 2020.

SERVICE & OUTREACH:

Member of Student Association in University of Jinan	2014-2015
Member of Psychological Development Association in University of Jinan	2014-2015
Chair of Information and Management System Committee in the University of Jinan	2016~2017
Member of Student Association in University of Chinese Academy of Science	2018-2019
Commissary in charge of general affairs in School of Nuclear Science and Technology in University of Chinese Academy of Science	2018-2019
Manager of football and basketball team in School of Nuclear Science and Technology in University of Chinese Academy of Science	2018-2019
Member of Choir team of School of Nuclear Science and Technology in University of Chinese Academy of Science	2018-2019
Member of Choir team of China Spallation Neutron Source	2019-2020
Instructor in the Chinese Academy of Sciences Public Science Day	2021.5

Instructor in the Chinese Academy of Sciences Public Science Day	2023.5
Volunteer ORNL Team UT-Battelle's need "Litter Clean Up activity in Concord Park off Northshore Drive”	Mar. 16, 2024
Volunteer ORNL Team UT-Battelle's need "Litter Clean up at Haw Ridge”	Mar. 30,2024
Member, American Physical Society	Science 2024-
Member, American Chemical Society	2024
Volunteer ORNL Team UT-Battelle's need LItter Clean Up Day-Scarboro Community in Anderson County	Dec. 7, 2024

Reviewer for ACS materials & interface, ACS applied energy materials, Physical Review B, Applied Sciences, Journal of physical chemistry, Materials, Physica, Thermo.

HONORS & AWARDS

Best student award in Chinese Academy of Sciences	2022~2023
Director's Scholarship (excellence award) in the Institute of High Energy Physics	2022
National doctoral Scholarship in China	2022
Best students award in the Application of Machine Learning in Condensed Matter Physics (NSFC)	2022
Top student award in Chinese Academy of Sciences	2021~2022
First award of Doctoral Scholarship	2021
Best student award in Chinese Academy of Sciences	2020~2021
Second award of Doctoral Scholarship	2020
Doctoral Scholarship of Dongguan Research Department, IHEP, CAS	2020
The silver award in chorus contest at Songshan Lake	2019
Best student award in Chinese Academy of Sciences	2018~2019
The second-class award in chorus contest at Chinese Academy of Sciences	2018
The second-class award in Shandong Province for the National College Students Mathematical Modeling Contest	2016