REHMAN SHAFIQ UR

POSTDOCTRAIL FELLOW

Personal information

Name
Shafiq Ur Rehman
Birthdate
04/02/1988
Gender
male
Residence
Shenzhen, Guangdong province, China
Nationality
Pakistan
Martial status
married

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- https://github.com/dashboard
- Shafiq Ur Rehman

Profile

I am a computational materials scientist. Studying material properties with first principles calculations, ab-initio/classical molecular dynamic simulations and machine learning. I am looking for research and teaching opportunities to utilized and enhanced my skills in the digital and AI era.

Experience

2022 - 2024
Yangtze River Delta Institute of University of electronic Science and Technology of China
Huzhou city, Zhejiang province, China,
Postdoctoral research fellow
Thesis: Optoelectronic and photo/electro-catalytic properties of 2D materials

2021 - 2022
Department of Materials science and Engineering, Southern University of Science and Technology of China
Shenzhen city, Guangdong, China,
Research associate
Thesis: Optical excitation, doping and defects in 2D composite materials

2018 - 2020
College of Optoelectronic Engineering, Shenzhen University
Shenzhen city, Guangdong, China,
Postdoctoral research fellow
Thesis: Optoelectronic properties of 2D heterojunctions and Li & Na ion battery applications

Education

2014 - 2018
PhD/computational Condensed Matter Physics
University of Science and Technology of C hina (QS world ranked: 78th), Hefei, Anhui Province
Thesis: First principles studies of 2D heterojunctions for optoelectronic and energy storage devices.

2011 - 2014
M.Phil./Physics
Hazara University, Mansehra, Pakistan
Thesis: Density functional theory study of nanomaterials and quantum dots for optoelectronic and spintronic application.

2009 - 2011 **MSc/Physics (Gold Medallist)**
Hazara University, Mansehra, Pakistan
Thesis: Theoretical investigations of Nanomaterials for spintronic applications

2007 - 2009 **BSc/Physics**
University of Peshawar, Pakistan
Major subjects: Mathematics/Physics

Professional Education

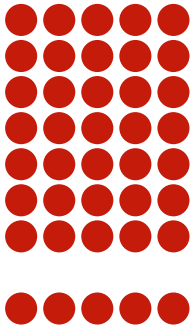
2010 - 2012 **Bachelor in education**
Northern University, Nowshera, Pakistan
Description: Methodologies for teaching of Physics and mathematics

2014 - 2015 **Chinese language course**
Anhui Normal University, Wuhu, China
Description: Learn Chinese language course

Skills

Skill group

VASP code
LAMMPS
Materials studio
Quantum espresso
Mathematica
python/linux
Machine learning/Scikit learn
COMSOL code



Achievements

Chinese government scholarship award (2014-2018)
Fully funded award for PhD studies in USTC, China

Gold medal award in MSc Physics (2011)
I got highest score (CGPA: 3.9/4) in MSc Physics, among the successful candidates and awarded Gold medal.

award in 7th Physical academic form of USTC (2017)
Got 3rd position in PhD topic presentation's competition

Best reviewers awards
I have got best reviewer award from IOP society, UK

Research associate professor award
Based on academic achievements, I got this award from Zhejiang province, China.

Interests

Research Interests

(1) First-principles calculations and predictions of functional materials, focusing on their electronic, optical and catalytic properties, lattice dynamics, defects, and growth dynamics
(2) Development of new computational methods
(3) Using machine learning tools to predicts new functional materials
(4) Using finite element analysis in COMSOL to study device performances and efficiency.

Professional services (Reviewer)

Journal of Physics: condensed matter
Journal of Material Research express
Journal of Alloys and Compounds
Nanotechnology
Journal of International energy Research
Journal of Saudi chemical society, Physica scripta

Teaching course (lectures)

2018 - 2020 **COMPUTATAIONAL MATERIALS SCIENCE**
Shenzhen university, Shenzhen, Guangdong, China
Course contents: Introduction of computational materials science, density functional theory and basic concept of solids. Basic knowledge of VASP code and hands on practices. Installations and use of SSH tools, visualisation tools like materials studio, vesta, VASPKIT etc. Developing codes in Mathematica/ python for analysis of DFT data. Properties calculations such as electronic, optical, vibrational, thermodynamic, thermoelectric and ferroelectric etc with VASP code. Classical molecular dynamic (LAMMPS) and ab-initio molecular dynamic simulations.

2012 - 2014 **SOLID STATE PHYSICS AND QUANTUM PHYSICS**
Hazara University, Mansehra, Pakistan
Introduction of solid state Physics, Quantum Physics, Electrodynamics

2011 - 2012 **PHYSICS/MATHEMATICS**
Tameer Millat public school and college, Mansehra, Pakistan
Basic school and college level teaching of Physics and maths.

Publications

Journal articles

Shafiq Ur Rehman, J. W. Wang, G. Wu, J. Xian, and Nasir Mahmood Unravelling the photocatalytic potential of transition metal sulfide and selenide monolayers for overall water splitting and photo-corrosion inhibition J. Mater. Chem. A, 12 (2024),6693–670. (IF: 11.9; JCR=1)

Shafiq Ur Rehman, Q. Sun, J. Wang, W. Lv, A. Azim, Y. Liu, J. Xian and N. Mahmood, In-plane heterostructures of transition metal dichalcogenide monolayers with enhanced charge separation and effective overall water splitting, Int J Hydrogen Energy, 80 (2024),280-288. (IF: 8.1; JCR=1)

Shafiq Ur Rehman and Ling Zhu Computational insight of ZrS2/graphene heterobilayer as an efficient anode material Appl.Surf. Sci., 551 (2021) 149304-9. (IF: 7.15; JCR=1)

Shafiq Ur Rehman and Ling Zhu Realization of Noble Heterobilayers with Enhanced Optoelectronic Properties Appl.Surf. Sci., 505 (2020) 144-530. (IF: 7.15; JCR=1)

Shafiq Ur Rehman and Ling Zhu Orientation Dependent Electronic and Optical Properties of ZnS Nanowires and ZnS-Si Core-Shell Nanowires Appl.Surf. Sci., 486 (2019) 539-545. (IF: 7.15; JCR=1)

Shafiq Ur Rehman and Z.J. Ding Enhanced Electronic and Optical Properties of Three TMDCs Heterobilayers, Phys. Chem. Chem. Phys., 20(2018) 16604-16614. (IF:4.5, JCR=1)

Shafiq Ur Rehman, H.M. Li and Z.J. Ding Structural and Electronic Properties of CdSe/ZnS and ZnS/CdSe Core/Shell Nanowires via First Principles Study J. Phys. Chem. Solids 116 (2018) 37-42. (IF: 4; JCR=2)

Shafiq Ur Rehman, Z.Y. Li, H.M. Li and Z.J. Ding Band Gap Modulation and Indirect to Direct Band Gap Transition in ZnS/Si and Si/ZnS Core/Shell Nanowires Physica B 524 (2017) 163-172.
Shafiq Ur Rehman* et al, Optoelectronic Properties of MoS2-ReS2 and ReS2-MoS2 Heterostructures, Physica B 577 (2020) 411809-18.

Shafiq Ur Rehman* et al, Structural, electronic, optical and thermoelectric analysis of perovskites XRuO3 (X=Ca, Sr) Physica B, 614 (2021) 412962-8.

Shafiq Ur Rehman and Ling Zhu First principle study of new W2N monolayer: a promising candidate for Li+ ion batteries Int. J. Electrochem. Sci., 14 (2019) 3070 – 3080.

M. Hafeez, Shafiq Ur Rehman, A. S. Saleemi, M. Saeed and Z. Ling, Role of substrate interface energy in the synthesis of high-quality uniform layered ReS2 Appl.Surf. Sci., 493 (2019) 1215–1223. (IF: 7.15; JCR=1)

Muhammad Hafeez, Awais siddique saleemi, Shafiq Ur Rehman, Muhammad Adrees, Irshad A Mir and Ling Zhu CVD growth of layered Cr2O3 hexagonal Flakes for optoelectronic applications Appl.Surf. Sci. 536, 147713 (2021) (IF: 7.15; JCR=1)

Publications

Journal articles

M. Idrees, H. U. Din, Shafiq Ur Rehman, M. Shafiq, Yasir Saeed, H. D. Bui, Chuong V. Nguyen and Bin Amin, Electronicproperties and enhanced photocatalytic performance of van der Waals heterostructures of ZnO and Janus transition metal dichalcogenides, Phys. Chem. Chem. Phys., 2020,22, 10351-10359. (IF: 4.5; JCR=1)

S. Ali, Shafiq Ur Rehman and Z.J. Ding, Stable Plasmon Excitations in Quantum Nanowires Phys. Plasma 25 (2018) 082115.

M. Kiani, A. B. Kiani, S. A. Khan, Shafiq Ur Rehman, Q. Khan, A. S. Saleemi, A. Jalil, Z. Ling Facile synthesis of Gd and Sn co-doped BiFeO3 supported on nitrogen doped graphene for enhanced photocatalytic activity J. Phys. Chem. Solids 130 (2018)222-229. (IF: 4; JCR=2)

W. Liu, Y. Xie, T. Chen, Shafiq Ur Rehman, L. Zhu Rationally designed mesoporous In2O3 nanofbers functionalized Pt catalysts for high-performance acetone gas Sensors Sens. Actuators B Chem. 298 (2019) 126871-9. (IF: 7.5; JCR=1)

Irshad A. Mir, Mansoor A. Bhat, Zahir Muhammad, Shafiq Ur Rehman, M. Hafeez, Qasim Khan and Z. Ling Differential and Comparative Sensing Modes of AIS and AIS@ZnS Core-Shell Quantum Dots towards bioanalytes J. Alloy. Comp., 811 (2019) 151688-7. (IF: 6.2; JCR=1)

Sachin Kumar, Irshad Ahmad Mir, Mohan Chandra Mathpal, Zahir Muhammad, Shafiq Ur Rehman and Ling Zhu One-step hydrothermal synthesis of high surface area m-ZrO2 nanorings with lower band gap, blue emission and high photocatalytic activity Journal of Materials Science: Materials in Electronics, 30 (2019), 15923-15927.

Awais Siddique Saleemi, Muhammad Saeed, Muhammad Hussan, Shafiq Ur Rehman, Muhammad Hafeez, Shahid Mehmood, M. Aurang Zeb Gul Sial and Shern-long Lee Anomalous Non-Linear to Linear Shift in Magnetoresistance of Amorphous Carbon Films Crystals 9 (2019), 618-10.

W. Uddin, S. Rehman, M. Adanan Aslam, Shafiq Ur Rehman, M. Wu, M. Zhou Enhanced Microwave Absorption from the Magnetic-Dielectric Interface: A Hybrid rGO@Ni-Doped MoS2 Materials Research Bulletin, 130 (2020), 110943. (IF: 4.7; JCR=2)

Shah Khalid, Rabah Khenata, Yue Ma, Xiaoliang Sun, Gui Wu Lu, Wenqi Huang, Shafiq Ur Rehman Understanding of Structural, Electronic and Optical Properties of CuXY2 (X=Si, Ge, Y=P, As): A DFT + U Approach Optik, 166(2018), 169-176.

Muhammad Saeed, Izaz Ul Haq, Shafiq Ur Rehman, Akbar Ali, Wajid Ali Shah, Qasim khan and Imad khan, Optoelectronic and elastic properties of metal halides double perovskites Cs2InBiX6 (X=F, Cl, Br, I), Chin. Opt. Lett., 19, 030004 (2021).

Sajjad Ali, Rashid Iqbal, Azim Khan, Shafiq Ur Rehman, and Muhammad Haneef First-Principles Study of The Stability and Catalytic Performance Single-Atom Catalysts Supported on Doped and Defective Graphene for CO2 Hydrogenation to Formic Acid ACS Appl. Nano Mater. 2021, 4, 6893−6902. (IF: 5.097; JCR=1)

Publications

Journal articles

Wei Liu, Yu Zheng, Zhe Wang, Zhixun Wang, Jiao Yang, Mengxiao Chen, Miao Qi, Shafiq Ur Rehman, Perry Ping Shum, Ling Zhu, and Lei Wei Ultrasensitive Exhaled Breath Sensors Based on Anti-Resonant Hollow Core Fiber with In Situ Grown ZnO-Bi2O3 Nanosheets Adv. Mater. Interfaces 8 (2021) 2001978-9. (IF: 6.2; JCR=2)

Junaid Khan, Shah Khalid, Waqar Uddin, Rabah Khenata, Maaz Khan, Shafiq Ur Rehman, Munir Ahmad, Shuangxi Wang, Wenqi Huang, S. Bin Omran, Muhammad Fawad, A new approach to study combination mixture organic solvent ethylene carbonate with lithiumion for alkali-ion battery: A density functional theory Mater Sci Technol. 11 (2021) 1672-1677. (IF: 8.14; JCR=1)

Ling Zhu, Shafiq Ur Rehman, Lin Zhang, Shaoqi Wu, Yuelin Xie and Xinzhong Wang The Structural stabilities and Band Gap Engineering of Core-Shell Nanowires Conf. Ser.: Mater. Sci. Eng. 490 (2019) 022021.

Maryam Kiani, Xiao-Qing Tian, Abdul Basit Kiani, Shafiq Ur Rehman, Sayed Ali Khan, Karim Kha, Aysha Khan Tareen, Qudrat Ullah Khan, Ikhtesham Mahmood A first principle study: Effect of tin substitution on magnetic properties of bismuth ferrite nanoparticles prepared by sol-gel synthesis method Inorganic Chemistry Communication 127 (2021) 108483.

Ruhumuriza Jonathan, Shafiq Ur Rehman, Feng Cao, Hui Xu, Xuejuan Ma, Junwei Wang, Yifan Liu, Yinghua Niu, Xian Jian and Nasir Mahmood, Low-cost and large-scale preparation of ultrafine TiO2@C hybrids for high-performance degradation of methyl orange and formaldehyde under visible light, Nanotechnology Reviews, 12 (2023), 20220556-11. (IF: 7.6; JCR=2)

Xingguang Fu, Dawei Zou, Gaobang Chen, Xiong He, Shafiq Ur Rehman, Na Wang, Yifan Liu, Xian Jian, Ultralight FeSiAl micro-flake flying with propylene to favor fast growth of carbon nanotube arrays at 99 % high-efficient conversion, J. Alloy. Comp., 960 (2023), 171057-12. (IF: 6.2; JCR=1)

Shafiq Ur Rehman* et al, High throughput computational screening of new two dimensional monolayers for overall water splitting, (ACS applied materials and interfaces, submitted) (IF: 8.3; JCR=1).

Patents

Chinese patents accepted

Shafiq Ur Rehman, Finite Element Analysis Method for Mass Transport and Chemical Reactions in Porous Cathodes to Improve Hydrogen Fuel Cell Efficiency, China patent, 2024, patent No. 2024106099175 (accepted).

Shafiq Ur Rehman , Finite Element Analysis Method and System for Light Emission and Quantum Efficiency of Light Emitting Diodes, China patent, 2024, patent No. 2024106099176 (accepted).

Conferences

Conferences

Shafiq Ur Rehman

Size Dependent Structural and Electronic Properties of CdSe/ZnS and ZnS/CdSe Core Shell Nanowires

20th International VACUUM Congress (IVC-20) Busan, Korea, Aug. 21-26, 2016.

Shafiq Ur Rehman

Indirect to Direct Band Gap Transition in ZnS/Si and Si/ZnS Core Shell Nanowires

The 1st USTC-FHI workshop on Frontiers of Advances Electronic Structure Methods, Hefei, China, Jun 14-18, 2016.

Shafiq Ur Rehman

Realization of Noble Heterobilayers with Enhanced Optoelectronic properties, international conference on Physics and networks, 26-28 Sept. 2019, Hilton Garden Inn Houston Westbelt, Houston, USA.

Shafiq Ur Rehman

Role of in plane interface in controlling exciton recombination and enhanced photocatalytic properties

UK-Canada Joint symposium on coordination Chemistry, May.29-June.2, St Andrews University, Scotland, UK.

References

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