



Shafiq Ur Rehman, Ph.D (USTC), China
Computational Physicist and materials science Engineer

Personal information

Name

Shafiq Ur Rehman

Birthdate

04/02/1988

Gender

male

Residence

Shenzhen, Guangdong province, China

Nationality

Pakistan

Marital status

married

Contact

🏠 Shenzhen, Guangdong, China

☎ 0086-13053041567

📠 0086-13053041567

✉ shafiqphy123@gmail.com

🔍 <https://shafiq1988.github.io/>

🎓 <https://scholar.google.com/citations?hl=en&user=OKauAU0AAAAJ>

🌐 <https://github.com/Shafiq1988/>

🐦 @peace128944512

Author of 37 articles.

Total citations: 950

H-index: 15

Profile

Expert in DFT, ab-initio/classical MD, and multiscale modeling to engineer 2D/inorganic materials for catalysis, clean energy, and optoelectronics. Skilled in high-throughput screening, defect dynamics, and heterojunction optimization to enhance charge transport and catalytic activity. Seeking roles to innovate sustainable materials via computational design and mentor simulation-experimental synergy.

Experience

● 2022 - 2024

Yangtze River Delta Institute of University of Electronic Science and Technology of China

Huzhou city, Zhejiang province, China, Postdoctoral research fellow

Dissertation: [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

Project: [Optical excitation, doping and defects in 2D composite materials.](#)

● 2018 - 2020

College of Optoelectronic Engineering, Shenzhen University

Shenzhen city, Guangdong, China, Postdoctoral research fellow

Dissertation: [Optoelectronic properties of 2D heterojunctions and Li ion battery applications.](#)

Education

● 2014 - 2018

PhD/Condensed Matter Physics

University of Science and Technology of China (QS world ranked: 78th), Hefei, Anhui Province, China.

Dissertation: [First principles studies of 2D hetero-structures for optoelectronic and renewable energy applications.](#)

● 2011 - 2014

M.Phil/Physics

Hazara University, Mansehra, Pakistan

Dissertation: [First principles study of optical and electronic properties of semiconductor nanomaterials.](#)

● 2009 - 2011

MSc/Physics (Gold Medallist)

Hazara University, Mansehra, Pakistan

Dissertation: [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

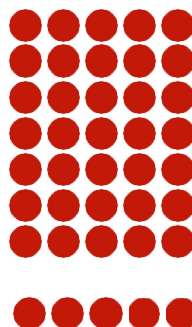
Chinese language course

Anhui Normal University, Wuhu, China

Description: Chinese language course (HSK-4)

Skills

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.

Research Interests

- (1) First-principles calculations of functional materials, focusing on structural electronic, optical and catalytic properties, lattice dynamic, defects and growth dynamics.
- (2) Ab-initio/classical molecular dynamic simulation for material's stability.
- (3) Combine DFT and ML to predicts material properties
- (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)

- | | |
|------|---|
| 2020 | COMPUTATAIONAL MATERIALS SCIENCE-1
<i>Shenzhen university, Shenzhen, Guangdong, China</i> |
| 2021 | COMPUTATAIONAL MATERIALS SCIENCE-2
<i>SUSTECH, Shenzhen, Guangdong, China</i> |
| 2012 | SOLID STATE PHYSICS AND QUANTUM PHYSICS
<i>Hazara University, Mansehra, Pakistan</i> |
| 2014 | PHYSICS/MATHEMATICS
<i>Tameer Millat public school and college, Mansehra, Pakistan</i> |

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, A. Samad, M. Saeed, B. Amin, M. Hafeez, I. A. Mir, Realization of Noble Heterobilayers with Enhanced Optoelectronic Properties, Appl.Surf. Sci., 505 (2020) 144-530. (IF: 7.15; JCR=1)

Shafiq Ur Rehman, M. Hafeez, W. Uddin, S. A. Khan, Q. Lu, L. Wei, M. Saeed, M. Sohail, S. Kumar, L. 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).

M. Hafeez, A. S. Saleemi, Shafiq Ur Rehman, M. Adrees, I. 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, Y. Saeed, H. D. Bui, Chuong V. Nguyen and Bin Amin, Electronic properties 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 nano-fibers 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).

S. Kumar, I. A. Mir, M. C. Mathpal, Z. 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.

A. Saleemi, M. Saeed, M. Hussan, Shafiq Ur Rehman, M. Hafeez, S. Mehmood, S. I. 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)

S. Khalid, R. Khenata, Y. Ma, X. Sun, G. W. Lu, W. 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.

M. Saeed, I. U. Haq, Shafiq Ur Rehman, A. Ali, W. A. Shah, Q. Khan and I. Khan, Optoelectronic and elastic properties of metal halides double perovskites Cs₂InBiX₆ (X=F, Cl, Br, I), Chin. Opt. Lett., 19, 030004 (2021).

S. Ali, R. Iqbal, A. Khan, Shafiq Ur Rehman, and M. 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

W. Liu, Y. Zheng, Z. Wang, Z. Wang, J. Yang, M. Chen, M. Qi, Shafiq Ur Rehman, P. P. Shum, L. 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)

J. Khan, S. Khalid, W. Uddin, R. Khenata, M. Khan, Shafiq Ur Rehman, M. Ahmad, S. Wang, W. Huang, S. Bin Omran, M. 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)

M. Kiani, X. Q. Tian, A. B. Kiani, Shafiq Ur Rehman, S. A. Khan, Karim Kha, I. 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.

R. Jonathan, Shafiq Ur Rehman, F. Cao, H. Xu, X. Ma, J. Wang, Y. Liu, Y. Niu, X. 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)

X. Fu, D. Zou, G. Chen, X. He, Shafiq Ur Rehman, N. Wang, Y. Liu, X. 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).

J. Wang, W. Huo, Z. Peng, Z. Tian, Shafiq Ur Rehman, Z. Mei, Y. Niu, W. Lv, Enhancement of Ionic Conductivity in NASICON-Structured Li₃(Zr, Ti)₂(Si, Ge)₂PO₁₂: An Ab Initio Study, Advanced sustainable system, 9 (2025), 2401028.

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

Name, Prof. Dr. Jian Xian
Tel: +86-551-13648079577
jianxian@ustc.edu.cn

Name, Prof. Dr. Guangfu Luo
Tel: +86-755-88015991
luogf@sustech.edu.cn

Name, Prof. Dr. Liu Wei
Tel: +86-17663063778
wei@henu.edu.cn

Name, Prof. Dr. Nasir Mehmood
Tel: +447864647020
nasir.mahmood@rmit.edu.au