Hafiz Ghulam Abbas

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Education

Ph.D in Computational Physics March 2017 - February 2021
Department of Nanoscience and Technology Research Institute of Physics and Chemistry, Jeonbuk National University,Jeonju 561-756, Republic of South Korea.

Master in Physics 2013-2015
Lahore University of Management Sciences, Syed Babar Ali School of Science and Engineering, Lahore, Pakistan.

BS in Physics 2009-2013
Bahauddin Zakariya University, Department of Physics, Multan, Pakistan.

Professional Experience

- **Postdoctral Research Scholar;** Department of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science and Technology(DGIST), Republic of South Korea, March 2021.
- **Research Assistant;** Department of Chemistry, Research Institute of Physics and Chemistry, Jeonbuk National University, Republic of South Korea, March 2019 - December 2020.
- **Research Assistant;** Department of Nano and Advanced Materials, College of Engineering, Jeonju University, Republic of South Korea, March 2017 - February 2019.
- **Teaching Assistant;** Department of Physics, COMSATS University Islamabad, Pakistan, September 2016 - February 2017 .

Research Interests

Electronic Structure of layered Materials

In the light of the Density Functional Theory calculations, I study electronic structure, optical, carrier transport, X-ray Photoelectron Spectroscopy, piezoelectric, elastic, and multiferroic properties of layered materials. I also like to explore new novel layered materials structure prediction based on particle swarm intelligence method.

Computational Design for Sustainable Energy Conversion

I am also interested to explore CO_2 reduction,water oxidation (oxygen evolution reaction – OER) and reduction (hydrogen evolution reaction – HER), oxygen reduction reaction mechanisms.

Phase Transition in Metallic Glasses

Phase transitions in metellic glasses via *Ab-Initio* and Classical Molecular Dynamics simulations, classical potential parameterization based on force matching algorithm, radial distribution function, Structure factor, bond angle distribution, mean square displacement, Voronoi tessellation and HA index.

Computational Skills

Density Functional theory calculations.
Classical and Quantum-mechanical Molecular Dynamics Simulations.
Kinetic modeling using density functional theory calculations.
Structure predictions employing swarm intelligence based Algorithm.
Software packages **(VASP, LAMMPS, CALYPSO,FHI-aims Phonopy, Pyprocar, ASE, Material Studio, VNL, OVITO, and VESTA.)**
Programming languages **(FORTRAN 90 and Python.)**
Windows and Linux operating system.

Professional Activities and Service

Reviewer; Materials Chemistry and Physics; Condense Matter Physics; ACS Applied Materials and Interfaces; RSC Advances

Honors and Awards

Korean Research Foundation; Department of Nanoscience and Technology, Research Institute of Physics and Chemistry, Jeonbuk National University, Republic of South Korea, March 2017 - February 2021.

National Outreach Program; Department of Physics, Lahore University of Management and Sciences (LUMS), Lahore, Pakistan, 2013-2015.

Professional Associations

Member, Zakariyan Alumni Association of Physicists.
Member, LUMS Alumni Association of Physicists.

Conferences Attended

International Society of Electrochemistry 2021.
International Symposium Nano Korea 2021.
International Conference on Nano Convergence, January 2018.
International Symposium on Light and Life, Comsats Institute of Information Technology,Islamabad, 2015.
Conference on Quantum information,Lahore University of Management Sciences, Lahore, 2014.

List of Publications

1. **Abbas, H. G.**; Rehman, M. U. ; Hahn, J. R. Arsenic Carbide Allotropes Prediction: An Efficient Platform for Hole-Conductions, Optical and Photoelectrocatalysis Applications. *Apll. Surf. Sci.* **2021**,*562*, 150109.

2. **Abbas, H. G.**; Debela, T. T. ; Hahn, J. R.; Kang, H. S.Multiferroicity of Non-Janus MXY (X = Se/S, Y = Te/Se) Monolayers with Giant In-Plane Ferroelectricity. *J. Phys. Chem. C* **2021**, *125*, 7458–7465.

3. Kwak, I. H.; Kwon, I. S.; Debela, T. T.; **Abbas, H. G.**; Park, Y. C.; Seo, J.; Ahn, J.-p.; Lee, J. H.; Park, J.; Kang, H. S., Phase Evolution of $Re_{1-x}Mo_xSe_2$ Alloy Nanosheets and Their Enhanced Catalytic Activity toward Hydrogen Evolution Reaction. *ACS Nano* **2020**, *14*, 11995–12005.

4. Kwon, I. S.; Kwak, I. H.; Debela, T. T.; **Abbas, H. G.**; Park, C. Y.; Ahn, J.-P.; Park, J.; Kang, H. S. Se-Rich $MoSe_2$ Nanosheets and Their Superior Electrocatalytic Performance for Hydrogen Evolution Reaction. *ACS Nano* **2020**, *14*, 6295–6304.

5. **Abbas, H. G.**; Hahn, J. R.; Kang, H. S. Non-Janus WSSe/MoSSe Heterobilayer and Its Photocatalytic Band Offset. *J. Phys. Chem. C* **2020**, *124*, 381219. **(Selected as front Cover Article)**

6. **Abbas, H. G.** Hahn, J. R. Crystallization Mechanism of Liquid Tellurium from Classical Molecular Dynamics Simulation. *Mater. Chem. and Phys.* **2019**, *240*, 122235.

7. **Abbas, H. G.** Debela, T. T.; Hussain, S.; Hussain, I. Inorganic Molecule (O_2, NO) Adsorption on Nitrogen and Phosphorus Doped MoS_2 Monolayer Using First Principle Calculations. *RSC Adv.* **2018**, *8*, 38656-38666.

8. Kwon, I. S.; Kwak, I. H.; **Abbas, H. G.** Lee, Y.; Jung, G.; Yoo, S. J.; Kim, J.-G.; Park, J.; Kang, H. S. Intercalation of Aromatic Amine for the 2H-1T' Phase Transition of MoS_2 by Experiments and Calculations. *Nanoscale* **2018**, *10*, 11349-11356. **(Equal Contributor)**

9. Kwak, I. H.; Kwon, I. S.; **Abbas, H. G.**; Jung, G.; Lee, Y.; Park, J.; Kang, H. S. Stable Methylammonium-Intercalated 1T'-MoS_2 for Efficient Electrocatalytic Hydrogen Evolution. *J. Mater. Chem. A* **2018**, *6*, 5613-5617. **(Equal Contributor)**

10. Kwak, I. H.; Kwon, I. S.; **Abbas, H. G.**; Seo, J.; Jung, G.; Lee, Y.; Kim, D.; Ahn, J.-P.; Park, J.; Kang, H. S. Intercalated Complexes of 1T'-MoS_2 Nanosheets with Alkylated Phenylenediamines as Excellent Catalysts for Electrochemical Hydrogen Evolution. *J. Mater. Chem. A* **2019**,*7*, 2334-2343. **(Equal Contributor)**

11. Kwon, I. S.; Kwak, I. H.;**Abbas, H. G.**; Seo, H. W.; Seo, J.; Park, K.; Park, J.; Kang, H. S. Two Dimensional MoS_2 Meets Porphyrins Via Intercalation to Enhance the Electrocatalytic Activity Toward Hydrogen Evolution. *Nanoscale Commun.* **2019**, *11*, 3780-3785. **(Equal Contributor)**

12. Kwak, I. H.; **Abbas, H. G.**; Kwon, I. S.; Park, Y. C.; Seo, J.; Cho, M. K.; Ahn, J. P.; Seo, H. W.; Park, J.; Kang, H. S. Intercalation of Cobaltocene into WS_2 Nanosheets for Enhanced Catalytic Hydrogen Evolution Reaction. *J. Mater. Chem. A* **2019**, *7*, 8101-8106. **(Equal Contributor)**

13. Kwon, I. S.; Kwak, I. H.; Kim, J. Y.; **Abbas, H. G.**; Debela, T. T.; Seo, J.; Cho, M. K.; Ahn, J.-P.; Park, J.; Kang, H. S. Two-Dimensional MoS_2/Fe-Phthalocyanine Hybrid Nanostructures as Excellent Electrocatalysts for Hydrogen Evolution and Oxygen Reduction Reactions. *Nanoscale* **2019**, *11*, 14266-14275.

14. Kwak, I. H.; Kwon, I. S.; **Abbas, H. G.** Lee, Y. R.; Jung, G.; Debela, T. T.; Yoo, S. J.; Kim, J.-G.; Park, J.; Kang, H. S. Nitrogen-Rich 1T'-MoS_2 Layered Nanostructures Using Alkyl Amines for High Catalytic Performance of Hydrogen Evolution. *Nanoscale* **2018**, *10*, 14726.

15. Debela, T. T.; **Abbas, H. G.** Role of Nanosize Icosahedral Quasicrystal of Mg-Al and Mg-Ca Alloys in Avoiding Crystallization of Liquid Mg: Ab Initio Molecular Dynamics Study. *J. Non-Cryst. Solids* **2018**, *499*, 173-182.

16. Jang, S.; Shin, T.; **Abbas, H. G.**; Hahn, J. R.; Kang, H. S. Orientation-Specific Switching of Inelastic Electron Tunneling in an Oxygen–Pyridine Complex Adsorbed onto an Ag(110) Surface. *J. Chem. Phys.* **2019**, *151*, 114703.

17. Afira, M.;**Abbas, H. G.** Muhammad, R.; Atif, S. Directional Mechanical and Thermal Properties of Single-Layer Black Phosphorus by Classical Molecular Dynamics. *Chinese Physics B* **2018**, *27*, 017401.

18. Jung, C. S.; Kim, D.; Cha, S.; Myung, Y.; Shojaei, F.; **Abbas, H. G.** Lee, J. A.; Cha, E. H.; Park, J.; Kang, H. S. Two-Dimensional GeAs with a Visible Range Band Gap. *J. Mater. Chem. A* **2018**,*6*, 9089-9098.

19. Hussain, S.; Patil, S. A.; Memon, A. A.; Vikraman, D.; **Abbas, H. G.** Jeong, S. H.; Kim, H.-S.; Kim, H.-S.; Jung, J. Development of a $WS_2/MoTe_2$ Heterostructure as a Counter Electrode for the Improved Performance in Dye-Sensitized Solar Cells. *Inorg. Chem. Front.* **2018**, *5*, 3178-3183.