Dear Prof. Liping Yu,

Subject: **Post-Doctoral Research Candidate**

I have been fortunate to find information about this opportunity to join you at The University of Maine, while I was looking for research opportunities in the field of Theoretical and Computational materials designs. I have all the necessary qualifications and experience to successfully fulfill the requirements for this position. I hold Ph.D. (Physical Chemistry / Chemical Physics) form University of Science and Technology of China, Hefei, China (Ranked 89 in world) under supervision of Prof. Zhenyu Li. I am actively Involved in research with particular interests in density functional theory (DFT), FPL/APW+lo and pseudopotential methods. During my academic career I have been involved in different theoretical and experimental fields of physical chemistry. My research experiences range from quantum chemical calculations using density functional theory (DFT) of materials to managing and facilitating experimentalists during my job at Syed Baber Ali School of Science and Engineering, Lahore University of Management Sciences (SBA-SSE, LUMS).

I have authored papers published in reputable material science journals such as Advanced Functional Materials, Materials Today Energy and ACS Omega. I am also actively involved in contribution as a co-author to number of papers published in international reputable SCI journals. Up to now my research subjects varied form novel low dimensional **inorganic electride materials** to **ferromagnetic semiconductors** and **ceramic materials** for water splitting applications. Currently, I am advance tools for computational material design to draw a rational for novel inorganic 2D materials in the field of energy storage. In my most recent paper we predict a theoretical rational for B_3P-monolayer for Li ion and Na ion storage as a superior 2D inorganic anode material. For future I also have developed interest to carry on my research in the field of computational heterogeneous catalysis in for exploring and designing technologically important nanomaterial. I have always been interested in to explore surface chemical properties of materials which would help provide proof to concept results. I would like to take this opportunity available with you as a Postdoc to explore "2D materials for energy storage applications, using a combination of first-principles density functional calculations and machine learning techniques".

The increasing influence of computational models has enabled researchers to simulate the nanoscopic materials for studying atomistic interactions which dictate their physical and chemical properties. With this opportunity I would like to take advantage of advancement in computational power along with the advancing theoretical models describing nanoscopic material properties, particularly based on density functional theory (DFT). I will use my knowledge of chemical physics, and skills I have developed practicing DFT calculation using VASP quantum chemical simulation package, for understanding, highlighting and delivering rational theoretical 2D materials fulfilling the increased demand for inorganic 2D materials for energy storage applications. I expect our contribution would help to define achievable paths for fellow experimentalists.

Syed Muhammad Ghulam Abbas Shah Gilani
P.hD. Chemistry
(Physical Chemistry / Chemical Physics)
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Disbale

SYED MUHAMMAD GHULAM ABBAS SHAH GILANI
PHYSICAL CHMEISTRY/ CHEMICAL PHYSICS
UNIVERSITYOF SCINCE AND TECHNOLGY CHINA
HEFEI, ANHUI CHINA

PROFILE

Age: 32 (DOB: 16, Aug 1988)

A highly motivated, numerate, and reliable Ph.D. with a strong academic background, experience, conscientious and detail oriented.

Currently my research interest revolves around designing novel low dimensional materials by understanding their atomistic level properties through electronic structure theory in combination with first-principles calculations.
Special Interest:

- Inorganic two dimensional materials.
- Atomic level understanding of the reactions in ion battery.
- Design Principles for two-dimensional single-atom catalysts.

SKILLS

VASP, WIEN2k, CALYPSO, ATK Quantum Wise, Material studio, VESTA, , Design Expert, MS (Office, Excel, PowerPoint), Python, Windows Operating System, Installation Software, System Recoveries, Linux, Ubuntu, Projects formatting and presentation preparations on Coral Draw and Adobe Photoshop, PhotoScape, Internet & E-mail

PUBLICATIONS

Two-Dimensional B_3P monolayer a superior anode material for Li and Na ion batteries: A First principles study. **Ghulam Abbas**, Syed Muhammad Alay-e-Abbas, Amel Laref, Yu li, Wen-Xing Zhang. Materials Today Energy. (accepted)
https://doi.org/10.1016/j.mtener.2020.100486

Investigation of Structural, Electronic and Optical Properties of (V+P)-doped $BaZrO_3$ for Photocatalytic Applications using Density Functional Theory. Shaheen Akhtar, Syed Muhammad Alay-e-Abbas, Javaria Batool, Waqas Zulfiqar, Amel Laref, Ghulam Abbas, Nasir Amin. ***Journal of Physics and Chemistry of Solids,*** 2020, 109662.
https://doi.org/10.1016/j.jpcs.2020.109662

Recent Advances in Twisted Structures of Flatland Materials and Crafting Moiré Superlattices. **Ghulam Abbas,** Yu li, Huide Wang, Wen-Xing Zhang, Cong Wang and Han Zhang. June, 2020 (accepted, in production) ***Advanced Functional Materials***. 2020, 2000878
https://doi.org/10.1002/adfm.202000878

Theoretical investigation of thermodynamic and optoelectronic properties of Ce4+ doped $SrZrO_3$ ceramics: A DFT study. Syed Muhammad Alay-e-Abbasa, Muhammad Waqar Yousaf, **Ghulam Abbas**, Nasir Amina, Amel Laref. ***Ceramics International***. 2019, 45(15) 18281-18290.
https://doi.org/10.1016/j.ceramint.2019.06.040

Density Functional Theory Evaluation of Ceramics Suitable for Hybrid Advanced Oxidation Processes: A Case Study for Ce^{4+}-Doped $BaZrO_3$. S.M. Alay-e-Abbas, Farrukh Javed, **Ghulam Abbas**, Nasir Amin, And Amel Laref. ***Journal of Physical Chemistry C***. 2019, 123(10) 6044–6053
https://pubs.acs.org.ccindex.cn/doi/10.1021/acs.jpcc.8b12221

Obtaining intrinsically occupied free-space superatom states in an encapsulated Ca_2N nanotube. **Ghulam abbas**, Songtao Zhao, Zhenyu Li and Jinlong Yang. ***ACS OMEGA***, 2018, 3(9) 11966-11971.
https://pubs.acs.org/doi/pdf/10.1021/acsomega.8b01575?src=recsys

Applications Hardware installation, recoveries, Networking Typing speed 35 wpm.

EDUACTION

PhD• 2019 • Physical Chemistry / Chemical Physics

UNIVERISTY OF SCIENCE AND TCECHNOLOGY CHINA, HEFEI CHINA.

M.Phil. • 2014 • Physical Chemistry

UNIVERSITY OF AGRICULTURE, FAISLABAD PAKISTAN.

BS hons. • 2012 • Chemistry

GOVERNMENT COLLEGE UNIVERISTY FAISALABAD, PAKISTAN.

LANGUGAE

I can speak, read, write, and understand proficiently following languages.
English, Urdu, Punjabi
(Chinese language Beginner level)

INTERPERSONAL ATTRIBUTES

Punctual & professional Approach.
Hard Working.
Excellent interpersonal communication skills.
Passionate about Photography.

First-principles evaluation of electronic and optical properties of (Mo, C) codoped BaHfO3 for applications in photocatalysis. S. Akhtar,S. M. Alay-e-Abbas, **S. M. GhulamAbbas**, M. Imran Arshad, Javaria Batool, and Nasir Amin. ***Journal of Applied Physics.*** 2018, 123(16) 161569.
https://aip.scitation.org/doi/pdf/10.1063/1.5010969?class=pdf

Ab initio calculations of Half-metallic ferromagnetism in Cr-doped MgSe and MgTe semicondcutors. N. A. Noor, S. M. Alay-e-Abbas, M. U. Shoib, **S.M. Ghulam Abbas** and A. Shaukat. ***Journal of Magnetism and Magnetic Materials***. 2015, 374: 164–172.

Ab initio study of electronic structure and magnetic properties in ferromagnetic Be1-xMnxSe and $Be_{1-x}Mn_xTe$ alloys, N. A. Noor, S. M. Alay-e-Abbas, Y. Saeed, **S. M. Ghulam Abbas** and A. Shaukat. ***Journal of Magnetism and Magnetic Materials***. 2013, 339: 11–19.

Structural, electronic, magnetic and optical properties of feromagnetic Pb 1-x Eu x Se and Pb 1-x Eu x Te alloys (x= 0, 0.25, 0.50, 0.75 and 1) S. M. Alay-e Abbas, S. Younas, S. Hanif, M. Sharif, Iqbal Hussain, **S. M. Ghulam Abbas** and A. Shaukat. ***International Journal of Modern Physics* B**. 2013, 27(19) 1350100.

WORK EXPERIENCE

SHENZHEN UNIVERISTY,

POSTDOCTRAL RESEARCH FELLOW

LUMS DEPARTMENT OF CHEMISTRY AND CHEMICAL ENGINEERING, SYED BABER ALI SCHOOL OF SCIENCE AND ENGINEERING, LAHORE UNIVERSITY OF MANAGEMENT SCIENCES

Lab Facilitator Dpt. Of Chemistry (2014-2015)

LA SALLE HIGH SCHOOL AND COLLEGE

Lecturer of Chemistry (2013-2014)

GOVT. MUNICIPAL DEGREE COLLEGE FAISALABAD

Lecturer of Chemistry (2012-2013)

SCHOALRSHIPS

1. Winner of Presidents CAS TWAS Fellowship award 2015.
2. University of Agriculture, Faisalabad tuition fee waiver for special person.

PROJECTS COMPLETED

- First principal study of novel alkaline earth metal sub nitrides.
- Microwave assisted Photocatalytic desulphurization of coal.

REFRENCES

Professor Zhenyu Li
http://staff.ustc.edu.cn/~zyli/resume.html
zyli@ustc.edu.cn

Professor Ijaz Ahmad Bhatti
http://uaf.edu.pk/EmployeeDetail.aspx?userid=333
ijazchem@yahoo.com

Professor Irshad Hussain
Lahore University of Management Sciences
https://lums.edu.pk/lums_employee/1922
ihussain@lums.edu.pk