

MASOOD YOUSAF, Ph.D. PHYSICS

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STRENGTHS

- Experience of Designing & Executing Research Projects
- Experience of Handling Surfaces & Interfacial Processes
- Expertise with Electronic Structure Codes (Quantum ESPRESSO, WIEN2k, VASP)
- Experimental Collaborations (Raman & IR Spectra, XPS, Prediction of Experimental Conditions)

QUALIFICATION

Ph.D Physics

Universiti Teknologi Malaysia

Research Area

Computational Simulation and Modelling of Materials

2014

EMPLOYMENT HISTORY

- **Postdoctoral Researcher** (01/11/2014- Present)
IBS Center for Multidimensional Carbon Materials (CMCM) Physics, Ulsan National Institute of Science and Technology (UNIST), Korea
- **Visiting Researcher** (01/07/2014 – 30/09/2014)
Department of Physics, Universiti Teknologi Malaysia (UTM)
- **Research Associate** (18/09/2013 - 28/02/2014)
Department of Physics, Lahore University of Management Sciences (LUMS)
- **Teaching Assistant** (SEM I Session 2012/2013)
Department of Physics, Universiti Teknologi Malaysia (UTM)
- **Lecturer of Physics** (08/08/2008 - 02/15/2012)
Punjab College Of Science, Lahore, Pakistan
- **Industrial Training** (10/06/2009 - 09/07/2009)
Ittehad Chemicals Limited

HONORS AND AWARDS

- **Academic Excellence Award (Alumni Award):** For the high achievements during the doctorate study program, awarded by Universiti Teknologi Malaysia. In conjunction with 53rd Convocation ceremony, 2014.
- **Best Postgraduate Student Award:** For the best student in Doctor of Philosophy (Physics) program, awarded by School of Postgraduate Studies (SPS), Universiti Teknologi Malaysia, 2014.
- Succeeded in winning consecutive **UTM International Doctoral Fellowship (IDF)** for Sem. I Session 2012-2013, Sem. II Session 2012-2013 and Sem. I Session 2013-2014.
- Certificate of appreciation (**Roll Of Honour**) for securing 1st class in M.Sc Physics.

RESEARCH EXPERIENCE

- Research experience on the activation of an unfavorable chemical processes by applying an electric field with an appropriate resonance frequency. The idea is to transfer energy through a harmonic electric pulse to design a particular surface chemistry.
- Exploring the energetics & dynamics of intercalated hydrogen at the metal-graphene interface. Hydrogenation treatment of single and few layers of graphene on various transition metal surfaces such as Cu, Pt, Pd, and Ni, aiming at obtaining ultrathin sp^3 -bonded carbon films is considered.
- My research work involves diverse calculations on the electronic structure and optoelectronic properties of various simple (such as binary phosphides and antimonides) and complex (such as AB_2C_4 type spinels and organic-inorganic hybrids) solid materials using numerical approaches at different level of sophistication. I have also calculated physical properties of materials at elevated conditions. I have calculated a number of structural, electronic and optical parameters and have developed equations for their prediction at above normal conditions.

COMPLETED RESEARCH PROJECTS

- Project entitled “Study of Structural and Electronic Properties of III-V Compounds by First Principles” under Foreign Academic Visitors (FAVG) Grant of Universiti Teknologi Malaysia. Grant No. JI3000077264D035; Amount Allocated= RM 40K (**Completed with publications**).

CERTIFICATES

- MATLAB for Scientists and Engineers
- Applied Numerical Methods for Engineers and Scientists using MATLAB
- Basic Steady State Simulation using CHEMCAD
- Heat Exchanger Design and Rating using CHEMCAD
- Implementation of QMS(ISO 9001:2008) in Process Industries
- Implementation of ISO 17025 for QA in Testing and Research Labs
- Energy Conservation and Sustainability
- Process Integration and Intensification
- HAZOP Study for Process Industries
- PRIMAVERA PROJECT MANAGER P3 (14-05-2010 to 28-05-2010 Institute of Quality & Technology Management, University of Punjab Lahore)

SCIENTIFIC ACTIVITIES ATTENDED

- **International Workshop On Materials Modeling And Simulations** (September 7-10, 2011, Department Of Physics, University Of Malakand, Pakistan).
- One month research visit to **Hakim Sabzevari University Iran** to study the development and implementation of modified approaches.

REVIEW SERVICES

Recognized reviewer of various international reputable journal such as

- Journal of Alloys & Compound
- Separation Science & Technology
- AIChE Journal

Some of the peer review activities can be viewed at <http://www.reviewerpage.com/Masood-Yousaf>

DOCTORAL THESIS EVALUATOR

- Manzar Ali, PhD Thesis entitled “Opto-electronic response of spinel compounds through modified becke-johnson exchange potential” Department of Physics, Hazara University Mansehra (11/05/2015).

TEACHERS TRAINING COURSE

- One month **teachers training course** from Punjab College Staff Training Institute.

MEMBERSHIPS

- Member of Pakistan Engineering Council
- Membership of Pakistan Institute Of Chemical Engineers (PICHE)

PUBLICATIONS

The articles published in reputed international journals are listed below and have attracted a number of external citations.

1. “Selective tuning of a particular chemical reaction on surfaces through electrical resonance: An ab initio molecular dynamics study”
Masood Yousaf, Dongbin Shin, Rodney Ruoff, and Noejung Park. Journal of Physical Chemistry Letters, 6 (2015) 5094–5099.
2. “Synergetic interplay between pressure and surface chemistry for the conversion of sp²-bonded carbon layers into sp³-bonded carbon films”
Y. Horbatenko, **Masood Yousaf**, J. Lee, T. H. Choi, R. S. Ruoff and N. Park. Carbon 106 (2016) 158–163.
3. “Carbon-heteroatom bond formation by ultrasonic chemical reaction for energy storage systems”,
H. T. Kim, H. Shin, I. Y. Jeon, **Masood Yousaf**, H. W. Cheong, N. Park, J. B. Baek, and T. H. Kwon. (Submitted to SCIENCE)
4. “Energetics and dynamics of intercalated hydrogen at the metal-graphene interface”,
Masood Yousaf et. al. (will be submitting soon)
5. “Role of graphene in water assisted oxidation of copper in relation to dry transfer of graphene”,
D. Luo, X. You, B. Li, X. Chen, H. Park, M. Jang, T. Y. Ko, K. Wong, **Masood Yousaf**, X. Chen, M. Huang, S. H. Lee, Z. Lee, H. Shin, S. Ryu, N. Park, R. R. Bacsa, W. Bacsa and Rodney S. Ruoff (Submitted to Chemistry of Materials)

6. “Exploring CVD Grown Graphene Membrane as Barrier to Hydrogen Permeation through Metals: Graphene Hydrogenation through Diffusion”
Pavel V. Bakharev, Manav Saxena, Ming Huang, Mandakini Biswal, Sunghwan Jin, Youngwoo Kwon, **Masood Yousaf**, Noejung Park & Rodney S. Ruoff
(will be submitting soon)
7. “Electronic, magnetic and optical properties of reduced hybrid layered complex Ni(pyz)V₄O₁₀ (pyz = C₄H₄N₂) by first-principles”
J. Munir, A. R. M. Isa, **Masood Yousaf**, H. R. Aliabad, Qurat-ul Ain, M. A. Saeed Journal of Magnetism and Magnetic Materials 416 (2016) 241–246.
8. “Structural, elastic, electronic, bonding, and optical properties of BeAZ₂ (A = Si, Ge, Sn; Z = P, As) chalcopyrites”
Shah Fahad, G. Murtaza, T. Ouahrani, R. Khenata, **Masood Yousaf**, S. Bin Omran, Saleh Mohammad. Journal of Alloys and Compound, 646 (2015) 211–222.
9. “Optoelectronic properties of XIn₂S₄ (X= Cd, Mg) thiospinels through highly accurate all-electron FP-LAPW method coupled with modified approximations”
Masood Yousaf, S. A. Dalhato, G. Murtaza, R. Khenata, M. Sajjad, A. Musa, H.A. Rahnamaye Aliabad and M. A. Saeed. Journal of Alloys and Compound, 625 (2015) 182–187.
10. “Prediction study of structural, electronic and optical properties of XIn₂S₄ (X = Hg, Zn) thiospinels under pressure effect”
Masood Yousaf, F. Inam, R. Khenata , G. Murtaza, A.R.M. Isa, M.A. Saeed. Journal of Alloys and Compound, 589 (2014) 353–363.
11. “Study of electronic band structure and optical parameters of X-Phosphides (X=B, Al, Ga, In) by modified Becke-Johnson potential”
Masood Yousaf, M. A. Saeed, R. Ahmed, M. M. Alsardia, A. R. M. Isa, A. Shaari. Communications in Theoretical Physics, 58 (2012), 777–784.
12. “An insight into the structural, electronic and transport characteristics of XIn₂S₄ (X=Zn, Hg) thiospinels using a highly accurate all-electron FP-LAPW+Lo method”
Masood Yousaf, M. A. Saeed, A. R. M. Isa, H. A. R. Aliabad, M. R. Sahar. Chinese Physics Letter, 30 (2013) 077402.
13. “Electronic band structure and optical parameters of spinel SnMg₂O₄ by modified Becke-Johnson potential”
Masood Yousaf, M. A. Saeed, A. R. M. Isa, A. Shaari, H. A. R. Aliabad. Chinese Physics Letter, 29 (2012) 107401.
14. “Ab initio study of optoelectronic properties of spinel ZnAl₂O₄ beyond GGA and LDA”
Masood Yousaf, M. A. Saeed, A. R. M. Isa, A. Shaari, H. A. R. Aliabad. International Journal of Modern Physics B, 26 (2012) 1250198.
15. “Study of electronic band structure and optical parameters of X-Antimonides (X=B, Al, Ga, In) by modified Becke-Johnson potential”
Masood Yousaf, M. A. Saeed, R. Ahmed, M. M. Alsardia, A. R. M. Isa, A. Shaari. Optoelectronics and Advanced Materials–Rapid Communications, 6 (2012) 902 - 910.
16. “Optoelectronic properties of pure and Co doped Indium Oxide by Hubbard and modified Becke Johnson Exchange Potentials”
H. A. R. Aliabad, M. Bazrafshan, H. Vaezi, **Masood Yousaf**, J. Munir, M. A. Saeed. Chinese Physics Letter, 30 (2013) 127101.

17. “Electronic and Optical Properties of Cubic Spinel CdX_2O_4 ($X=In, Ga, Al$) through Modified Becke—Johnson Potential”
A. Manzar, G. Murtaza, R. Khenata, **Masood Yousaf**, S. Muhammad and Hayatullah Chinese Physics Letter, 31, (2014) 067401.
18. “Structural, electronic, and optical properties of orthorhombic and triclinic $BiNbO_4$ determined via DFT calculations”
F. Litimein, R. Khenata, S. K. Gupta, G. Murtaza, Ali. H. Reshak, A. Bouhemadou, S. Bin Omran, **Masood Yousaf** and P. K. Jha. Journal of materials sciences, 49 (2014) 7809–7818.

INTERNATIONAL CONFERENCE PRESENTATIONS

1. “Designing a specific surface chemistry through electric field induced resonance”
Poster Presentation: Masood Yousaf
20th Nanotube Workshop (January 29-31, 2015, Muju Deogyusan Resort, Republic of Korea)
2. “Comparison of the electronic band structure profiles and optical properties of XIn_2S_4 ($X = Cd, Mg$) thiospinels”
Oral Presenter: Masood Yousaf
2nd International Science Postgraduate Conference (ISPC) (March10-12, 2014, Universiti Teknologi Malaysia)
3. “Study of electronic band structure and optical parameters of spinel $SnMg_2O_4$ beyond GGA and LDA”
Oral Presenter: Masood Yousaf
Joint International Conference on Nanoscience, Engineering and Management (BOND21) (August 19-21, 2013, Bayview Beach Resort, Penang, Malaysia)
4. “DFT Investigations of the Structural, Electronic and Optical Properties of XN ($X=Al, Ga, B, In$) compounds”
Oral Presenter: Masood Yousaf
International Conference on Solid State Physics (December 01-06, 2013, University of the Punjab, Lahore, Pakistan)
5. “Step by step approach in science”
Oral Presenter: Masood Yousaf
The 3rd Fiqh Science & Technology Seminar (May 19-20, 2012, Universiti Teknologi Malaysia)
6. “Study of electronic band structure and optical parameters of spinel $ZnAl_2O_4$ by modified Becke-Johnson potential”
Oral Presenter: Masood Yousaf
4th International Conference on Solid State Science and Technology (December 18-20, 2012, Melaka Malaysia)
7. “Opening of New Paths for Kinetically Limited Chemical Processes using Resonating E-field”
Oral Presenter: Masood Yousaf
The 10th International Conference on New Diamond and Nano Carbons (May 22-26, 2016, Xi’an Shaanxi, China)