

Dr Sardar Sikandar Hayat (I.F =150)

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Education

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|-----------------------------------|--|
| ➤ PhD (Physics) [2004-08] | Pakistan (IUB)/USA (University of Central Florida, Orlando, FL, USA) |
| ➤ M.Sc (Physics) [2001-03] | The Islamia University of Bahawalpur |
| ➤ B.Sc [1997-99] | The Islamia University of Bahawalpur |
| ➤ F.Sc [1995-97] | Govt. Khawaja Fariad College of RYK |
| ➤ S.S.C [1992-94] | Govt. Colony H/S Liaquatpur |

Personal

Father's Name	Noor Ahmad
Date & Place of Birth	July 20, 1978, Pakistan
CNIC#	31302-2146976-7
Marital Status	Married
Nationality	Pakistani
Languages	English, Urdu, Punjabi and Saraiki

Area of Research

- Molecular Dynamics studies of phenomena at the surfaces, nanostructures, diffusion, and vibrational dynamics.
- Thermal properties such as specific heat, thermal coefficient of expansion, structure factor, and melting temperature.
- Crystal defects such as point and planar defects in bulk crystals of metals and alloys and interactions of defects with the interfaces.
- Atomistic study of cluster diffusion at compact and complex solid surfaces (with steps and kinks); and epitaxial layer growth at the surfaces.
- First principle studies of charge density and band structures in the case of Metals and binary compounds.

PhD Thesis Title

“Computer Simulation of Planar Defects in Crystals of Metals using Molecular Dynamics”

Scientific Activity

Chief Organizer of two-day workshop on **New Trends in Materials Modelling** in September 23rd, 24th 2024 at the Department of Physics, IIU

Professional Experience (Research and Teaching > 20 Years)

Institution/Organization	Position /Job Title	Period	
		From	To
International Islamic University Islamabad	Associate Professor	05 – 03 – 2024	Continue
Bahauddin Zakariya University Multan	Professor	06 – 04 – 2023	04 – 03 – 2024
International Islamic University Islamabad	Associate Professor	30 – 08 – 2018	05 – 04 – 2023
Hazara University, Mansehra	Assistant Professor (TTS)	04 – 11 – 2010	30 – 08 – 2018
Hazara University, Mansehra	Lecturer	04 – 03 – 2009	03 – 11 – 2010
IUB Bahawalpur	Research and V. Lecturer	26 – 042 – 2008	03 – 03 – 2009
University of Central Florida (USA)	V. Researcher	20 – 09– 2007	25 – 02 – 2008
IUB Bahawalpur	Research Student of PhD and Visiting Faculty	20 – 04 – 2004	19 – 09 – 2007

Teaching Expertise (Graduate and Under Graduate level)

1. Solid-State Physics (I &II)
2. Materials Science (I &II)
3. Classical Mechanics
4. Advanced Mathematical Methods of Physics
5. Computational Physics
6. Atomic & Molecular Physics
7. Condensed Matter Physics
8. Research Methodology
9. Surface Physics
10. Modern Physics
11. Mechanics
12. Waves and Oscillations

Professional Responsibilities

- By default, member of BOS, BOF, Academic Council, and Senate of Bahauddin Zakariya University Multan.
- Member of Departmental Board of Studies, Department of Physics, Ghazi University, Dera Ghazi Khan, 04/11/2021 to 5/4/2023
- Member of Departmental Board of studies, IIUI, 31/08/2018 to 05-/04/202/3
- Member of Subject Selection Committee, IIU in Spring 2020
- Member of Departmental DTRC, IIUI, 28/01/2019 to 20/04/2021
- Convener of Departmental graveness committee, HU, 21/7/2016 to 30/8/2018
- Departmental Focal Person of Laptop Scheme, HU, 21/7/2016 to 30/8/2018
- Member of departmental Board of studies, HU, 21/7/2016 to 30/8/2018
- Member of the departmental committee for utility and maintenance, HU, 21/7/2016 to

30/8/2018

- Member of Departmental comprehensive examination committee for PhD, HU, 07/09/2010 to 30/8/2018
- Coordinator of general activities at the Department of Physics, Hazara University, 07/09/2010 to 30/8/2018
- In-charge of the computer lab

National/International Collaborations

- Computational Lab., Department of Physics, University of Central Florida, Orlando, Florida 32816, USA.
- LMPM, Mechanical Engineering Department, University of Sidi Bel Abbès, Sidi Bel Abbès 22000, Algeria.
- Institute of Science and Technology, University of Ain Temouchent, BP 284 RP, Ain Temouchent, 46000, Algeria.
- National Institute of Laser and Optonics, Nilore, Islamabad, 45650 Pakistan
- Department of Physics, Riphah International University, Islamabad, Pakistan
- Department of Physics, Govt. College University Faisalabad, Faisalabad 38000, Pakistan.

Skills

- Strong knowledge and research experience in Molecular dynamics technique
- Strong Programming expertise in the Fortran language
- Strong background in Crystallography, crystalline defects, thermal properties, and surface-diffusion
- Strong background in Materials Physics
- Expertise in running the Simulation Packages like Dynamo, Solids, Crystal, Lamps, Dyne86.
- Familiar with DFT and MC Simulations such as Win2K, WASP, SLKMC CPMD, and Quantum ESPRESSO.
- Expertise in working on Solaris, Linux, and Unix operating
- Strong expertise in office, origin and supporting software.
- Advanced English-level skills and excellent abilities in article writing, composing, and literature.

Distinction/Awards/Scholarship

- First Position in Secondary School Examination in Secondary School Liaquat Pur (1994)
- Indigenous Ph.D. Fellowship from Higher Education in 2004
- IRSP Scholarship from Higher Education in 2007.
- Gold Medal on the basis of Research Performance from Hazara University, Mansehra (2015)

Students Supervision

PhD Supervised at Physics (Hu and IIU)

	<i>Name of Student</i>	<i>Reg. No.</i>	<i>Title of Dissertation</i>
1	Qaiser Rafiq (IIU)	92-FBAS/PHDPHY/S19	<i>Simulation of d-Block Noble Metals Surfaces in the Presence of Small Homogeneous and Heterogeneous Adsorbed Islands</i>
2	Asif Zahir (IIU)	74-FBAS/PHDPHY/S16	<i>Quantum-coherence-assisted Optical Properties and Surface Plasmon Polaritons Drag via Quantum Dots-metallic Interfaces</i>
3	Adeel Ahma Awan (IIU)	Reg. No. 121-FBAS/PHD /F21	<i>Optimizing Visible Light Emission in Silicate Phosphors Through Defect Engineering and Lanthanide Doping: A DFT Study</i>
4	Mr. Noor Said (IIU)		<i>DFT Investigation of Optoelectronic and Magnetic Properties of Lanthanide-based Perovskite Oxides</i>
5	Dr. Zulfiqar Ali Shah (HEC Scholar) (HU)		<i>Study of Anharmonic Effects in the Presence of Adparticles at the Surfaces of Crystals of Nobel Metals</i>
6	Dr. Zakirur-Rehman (HU)		<i>Study of Thermal diffusive properties of d-Block transition Metals.</i>

MSc/BS Projects Completed at IIU

	<i>Name of Student</i>	<i>Registration No.</i>	<i>Title of Project</i>
1	Khuram and Nauman		<i>How natural Fountain develops in Hilly Areas</i>
2	M. Naveed M. Jumshaid Naeem	779-BAS/MSCPHY/F17 786-FBAS/MSCPHY/F17	<i>Study of piezoelectricity in Ferroelectrics at different temperatures</i>
3	Mubashir Mehboob, M. Anees M. Usama	1015-FBAS/BSPHY/F16, 1047-FBAS/BSPHY/F16 1055-FBAS/BSPHY/F16	<i>Computational Study of Electronic Structure of SrTiO₃ First Principle Calculation</i>
4	Irfan Ali Khan Mohsin Rasheed	965-BAS/MSCPHY/F18 987-FBAS/MSCPHY/F18	<i>Interaction of Points Defects With Twin Boundary of Crystal Structure</i>
5	Inam Ullah Khan, M. Abdullah Wajid Ali	1020-FBAS/BSPHY/F16, 1021-BAS/BSPHY/F16 1033-FBAS/BSPHY/F16	<i>Computational Study of Electronic Structure of PbTiO₃ First Principle Calculation</i>
6	Moeed ul Hassan, Shahzad Hussain, and Ahsan Tanveer	1474-FBAS/BSPHY/S19, 1498-FBAS/BSPHY/S19 1513-FBAS/BSPHY/S19	<i>DFT Predictions of Ga-doped AlSb for Optoelectronic Applications</i>
7	Ebtesam Sohail, M. Naveed Sultan, and M. Umar	1477-FBAS/BSPHY/S19, 1519-FBAS/BSPHY/S19 1523-FBAS/BSPHY/S19	<i>DFT Calculations of Tellurium Metalliod</i>
8	Muhammad Wazir, Moin Akbar, and Abdul Quyum	1470-FBAS/BSPHY/S19, 1508-FBAS/BSPHY/S19 1547-FBAS/BSPHY/S19	<i>DFT Calculations of Aluminum-Based Double Perovskite Materials</i>

9	Malik M. Kashif Arif, M. Numan Khan, and M Ismaeel	1797-FBAS/BSPHY/F19, 1707-FBAS/BSPHY/F19 1817-FBAS/BSPHY/F19	DFT Calculations of BaCu ₂ As ₂ and Alpha-BaCu ₂ Sb ₂ Materials
10	Arooj Fatima Syeda Eman Fatima	2230-FBAS/BSPHY/F21 2178-FBAS/BSPHY/F21	DFT Calculations of ZnO materials using CASTEP package
11	Laiba Farman Anam Nisar Akram Aleeshba Rani	2143-FBAS/BSPHY/F21 2144-FBAS/BSPHY/F21 2152-FBAS/BSPHY/F21	DFT Calculations of Ti ₂ and ZnO materials using material studio

MS Produced at the Physics Department of IIU

1	Adeel Ahmad Awan	551-FBAS/MSPHY/F18	Effect of C and N Co-doping on the Electronic Structure of SrTiO ₃
2	Mujeeb Ur Rehman	556-FBAS/MSPHY/F18	Computational Studies of Dynamics and Diffusion of Small Clusters of Zr on Cu(111) Surface
3	Mujahid Ali	568-FBAS/MSPHY/F 18	A First Principle Study of New Lead (Pb) Free Double Perovskite for Solar Cell Application
4	Muhammad Hashim	596-FBAS/MSPHY/F19	Effect of Crystal Defects on Thermal Properties of Pd and Pt: A Molecular Dynamics Approach
5	Assad Manzoor	600-FBAS/MSPHY/F19	Computational Studies of Anharmonic Effects at the Surface of Cu in the Presence of Ag Ad- particles
6	Syed Hannan Ali Bukhari	601-FBAS/MSPHY/F19	Interaction of Point Defects with Twin- boundaries in Silver Crystal
7	Shanawar Khan	621-FBAS/MSPHY/F19	Thermal Diffusive Behaviour of Cu and Zr Small Clusters on Al(111) Surface: A Molecular Dynamics Approach
8	Abdul Ghafar	640-FBAS/MSPHY/S22	First Principle Calculations of Structural, Electronic and Optical Properties of Cs ₂ AgLaX ₆ (X= Br, Cl, and I) Double Perovskite
9	Mr. Ali Afzal	667-FBAS/MSPHY/F22	Computational Study of Band Gap Engineering in Bi ₂ Te ₃ Through Zr and Ti Doping Using Density Functional Theory

MPhil Produced at HU (as a Supervisor)

S. #	Name of Student	Title of Thesis
9	Mr. Babar Shahzad Khan	Interaction of point defects with grain boundaries in metals
10	Mr. Zulfiqar Ali Shah	Theoretical Study of Anharmonic Effects Near the Interfaces of Crystals
11	Mr. Raheel Iqbal	Structural and magnetic properties metals and metallic Compounds
12	Mr. Zakir ur Rehman	Computational Study of Hetro-diffusion for FCC Metals
13	Mr. S. Siddique ur Rahman	Designing of Software for Three Phase Digital Energy Meter
14	Mr. Abul Raouf Malik	Study of the Efficiency of Phtosentizer Mediated Photodynamic Therapy on Cancerous Cell lines

15	Mr. Kashif Khan	<i>Theoretical Investigation of Structural and Electronic Properties of Semiconductors</i>
16	Mr. Imran Ullah	<i>Diffusion of Pd Islands on Pt(111) surface and Pt Islands on Pd(111) surface: A Molecular Dynamics Approach</i>
17	Mr. Humayun Khan	<i>Computational Study of monomer and dimer Diffusion on Pt(111) and Pd(111) surfaces at different temperature</i>
18	Mr. Asghar Ali	<i>Computational study of effect of crystal defects on thermal Properties</i>
19	Mr. H. Hussain	<i>Computer simulation of crystal defects in noble metals</i>
20	Mr. Sibghtullah	<i>First Principle Study of electronic and optical properties for $X^{II}-Y^{IV}-Z_2^V$ ($X=Zn, Cd$; $Z=P, As$) Chalcopyrites</i>
21	Mr. Waqas Gul	<i>Estimation of thermal properties of Pd and Pt A molecular dynamics approach</i>
22	Mr. M. Arif	<i>First Principle Study of XYZ half heusler compounds ($X=Li, Na, K$; $Y=Mg$; $Z=N, P, As, Sb, Bi$) Chalcopyrite</i>
23	Mr. Rashid Iqbal	<i>An ab-initio study of structural, electronic and magnetic properties of ThO_2 and CmO_2 compounds</i>
24	Mr. Sarfaraz Ahmad	<i>Structural and electronic tic properties of AmO_2 and PuO_2 Compounds</i>
25	Mr. Shah Saleemullah Sabir	<i>Study of dynamics of Cu and Ag trimer adatoms on compact surfaces at different temperatures</i>
26	Miss. Bushra Bibi	<i>Coalescence and deposition of silver nanoparticles on surface of silver</i>
27	Yasir Khan Abbasi	<i>Diffusion of Ag Clusters on different surfaces of Cu</i>
28	Mr. Wajid Ali	<i>Computational study of dynamics of small silver clusters on silver surface</i>
32	Mr. Wajid Ali	<i>Virtual simulation in external beam radiotherapy and comparison with 2D simulation</i>
33	Mr. Fawad Farooq	<i>Compositional Analysis of Archeological Artifacts using laser induced breakdown spectroscopy</i>
34	Mr. Sohaib Khan	<i>Simulation of ignition processes in AC plasma Torch</i>
35	Miss. Anum Pervez	<i>Computational Study of interaction between clusters on silver (111) surface</i>
36	Miss. Faiza Rehman	<i>Computational study of thermal diffusion dynamic behavior of 2-dimensional Cu small clusters on Cu(111) surface</i>
37	Muhammad Khuram	<i>Theoretical Study of Crystal defects in Nobel Metals</i>
38	Miss Shaista Anjum	<i>Study of Hetro-Epitaxy for Metals Using Molecular Dynamics Method</i>
39	Miss Humaira Naz	<i>Molecular Dynamics Study of Homo-Metallic Surface Behavio</i>

40	Mr. Fazal Ullah	<i>Computational study of the dynamics and diffusion of small Ag island on Cu(111) surface</i>
41	Mr. Zafar Javid	<i>Computational study of Thermal diffusion dynamic behaviour of two dimensional Ag-small clusters on Ag(111) surface.</i>
42	Mr. Asad Mehmood Ur	<i>Analysis of Plasma generated by laser induced breakdown Spectroscopy</i>
43	Mr. Muhammad Sulman	Study for Adsorption Si and Co on on Fe(111) and Solar Light Activity
44	Miss. Javeria	DFT Investigations of Pd Monomers on Pt(111): Insights into Atomic-scale Dynamics and Surface Properties
45	Mr. Fahad Mustafa	Computational Study of MgSiO ₃ Layered Perovskites Material for the Application of Storage Devices
46	Mr. Naeem Akhtar	DFT Calculations for BaSiO ₃ Oxide Material for the Application of Storage Devices
47	Mr. Ali Afzal	Computational Study of Band Gap Engineering in Bi ₂ Te ₃ Through Zr and Ti Doping Using Density Functional Theory
48	Mr. Habib Ur Rehman	Computational Study of Structural and Optoelectronic Properties of Mg _(1-x) Nb _x H ₂
49	Mrs. Smaira Habib	DFT Calculations of Hf and Sc doped ZnI ₂ S ₄ material
50	Mrs. Hajra Sadiq	DFT Calculations of Mg, Na, and K doped Cu ₂ Se material
51	Mrs. Haheer Bano	DFT Calculations of Fe and Cr doped MgTiO ₃ Peroskite material
52	Mrs. Ruqia Farooq	DFT Calculations for electrical and optical properties of Ru doped Mg ₂ SiO ₄ material

Examiner of PhD Students

	<i>Institution</i>	<i>Name of Student</i>	<i>Title of Project</i>
1	International Islamic University	Dr. Faisal Zaib	<i>Synthesis and Characterization of Coated and Uncoated Ferrite Magnetic</i>
2	Hazara University Mansehra	Dr. Sardar Siddique ur Rahman	<i>“Green Synthesis and Characterization of Fe₂O₃, ZnO and Ag Nanoparticles for Bio-Labeling and Biosensor Applications</i>
3	IUB	Dr. Kashif Ali	<i>Synthesis and Analysis of Physical Properties of Iron Oxide Based Nanocomposites</i>
4	IUB	Dr. Hur Abbas	<i>Effect of Doping and Coating on Magnetic and Optical Properties of NiO Nanoparticles</i>
5	IIU Islamabad	Dr. Muhammad Iftikhar	<i>Aerosol-Cloud Radiative Properties and its Impact on Climate</i>
6	Hazara University Mansehra	Dr. Munir Ahmad	<i>Synthesis of Metal Nanocomposites by Using Green and Chemical Route for Multiple Applications</i>
7	AIO University Islamabad	Dr. Sarfraz Ahmed	<i>Prediction of Structural, Electronic, and Optical Properties of 2D Materials from Group III-IV First Principals Study</i>
8	International Islamic University Islamabad	Dr. Muhammad Tayyab	<i>DFT Studies of Band-Gap Tuning of Two-dimensional Graphene, Molybdenum Di-sulfide and Molybdenum Di-bromide for Solar Cell Applications</i>
9	AIO University Islamabad	Dr. Zubeda Bhatti	<i>Designing of Solar Dryers for Small, Medium and Large Scale Dates in Khairpur, Sindh, Pakistan</i>
10	AIO University Islamabad	Dr. Muhammad Baqar Hussain Shah	<i>Study of ZnO-Based Composite Nanostructures (CNs) for Photocatalytic and Antibacterial Applications</i>

11	University of Malakand	Dr. Akbar Ali	<i>Ferroelectric and Magnetic Study of Corundum Double Oxides</i>
12	IU Bahawalpur	Dr. Saira Kiran	<i>"Reliability of Resistive Switching Material for RS Mechanism in RRAM Devices: DFT Study"</i>
13	Riphah International University	Dr. Muhammad Jawad	<i>Optimization Of Thermoelectric Properties Of Semiconducting Metal Oxides Using Density Functional Theory</i>

International Publications

1. **S. Sikandar Hayat**, M. A. Choudhry and S. A. Ahmad, *Effect of twin boundaries on melting of aluminum*, J Mater Sci (2008) 43:4915-4920. (ISSN NO. 22- 2461, I.F. 3.553) <http://dx.doi.org/10.1007/s10853-008-2715-x>
2. **S. Sikandar Hayat**, M. A. Choudhry, S. A. Ahmad, J. I. Akhter and A. Hussain, *Study of thermal properties of Ni using Embedded-atom method*, Ind J Pure & Appl Phys (2008) 46:771-775. (ISSN NO. 0019-5596, I.F.0.653)
3. A. Hussain, M. A. Choudhry, **S. Sikandar Hayat**, *Effects of ordering on thermal properties of Ni₃Al intermetallic alloy system: A Molecular dynamics approach*, Chinese Journal of Physics (2009) 47(3):344-355. (I.F.2.638)
4. **S. Sikandar Hayat**, M. A. Choudhry, A. Hussain, S. Alam, Sheikh A. Ahmad and I. Ahmad, *Nanoscale Relaxation near the Twin Interfaces of Palladium and Platinum*, Ind J Pure & Appl Phys (2009) 47:730-736. (ISSN NO. 0019-5596, I.F. 0.653)
5. **S. Sikandar Hayat**, Marisol Alcántara Ortigoza, M. A. Choudhry, and Talat S. Rahman, *Diffusion of Cu monomer and dimer on Ag(111) studied with the Molecular Dynamics Method*, Phys. Rev. B (2010) 82:085405-085415. (I.F. 3.772) <https://doi.org/10.1103/PhysRevB.82.085405>
6. Fekirini Hamida, Boualem Serier, Bouafia Farida, **S. Sikandar Hayat**, Bachir Bouiadjra Belabess. *Computation of the Stress Intensity Factors for Interface Cracks in Fibrous Composite*, American Scientific Publishers (2011)
7. Fekirini Hamida, Boualem Serier, Bouafia Farida, **S. Sikandar Hayat**, Bachir Bouiadjra Belabbes; *Effect of Density and Pointed Corner Degree of Pore on Local Stress in Welded Structures: Defect in Marine Structures*, American Scientific Publishers (2011)
8. F. Hussain, **S. Sikandar Hayat**, and M. Imran, *Interaction of small vacancy clusters with (114) twin-boundary in gold*, Physica B. (2011) 406:1060-1064 (ISSN: 0921-4526, I.F. 1.902) <https://doi.org/10.1016/j.physb.2010.11.001>
9. **S. Sikandar Hayat**, *Pop-up of atoms among copper 13-atom island on Ag(111)*, Computational material science, (2011) 50 (4):1485-1489. (ISSN: 0927-0256, I.F. 2.863) <https://doi.org/10.1016/j.commatsci.2010.12.003>
10. A. Hussain, **S. Sikandar Hayat** and M. A. Choudhry, *Ab-initio calculations of study of electronic structure and optical properties of TiAl alloy*, Physica B: Condensed Matter, (2011) 406:1961-1965 (ISSN: 0921-4526, I.F. 1.902) <https://doi.org/10.1016/j.physb.2011.02.065>
11. **S. Sikandar Hayat**, I. Ahmad, and M. A. Choudhry, *Diffusion of 6-atom Cu island on Cu(111) and Ag(111)*, Chinese Physics Letters (2011) 28(5):053601- 053604 (ISSN 0256-307X, I.F.1.066)
12. **S. Sikandar Hayat**, Zakir-ur-Rehman, Ghulam Hussain, and N. Hassan, *Copper 10-atom Island Diffusion on Ag(1 1 1) Surface*, Chinese Journal of Physics (2011) 49(6):1264-1272 (ISSN: 0577-9073, I.F.2.638)
13. M. Atif, R. Malik, M. Fakhar-e-Alam, **S. Sikandar Hayat**, S. S. Z. Zaidi, R. Suleman, and M. Ikram, *In Vitro studies of Phtotfrin[®] mediated photodynamic therapy on human Rhabdomyosarcoma cell line (RD)¹*, Laser Physics (2012) 22(1):286-293; <https://doi.org/10.1134/S1054660X11230010> (ISSN: 1054-660X, I.F. 3.605)

14. M.Atif, R.Malik,M.Fakhar-e-Alam, **S. Sikandar Hayat**, S.S.Z.Zaidi,R.Suleman,andM. Ikram, *Erratum: In Vitro studies of Phtotfrin[®] mediated photodynamic therapy on human Rhabdomyosarcoma cell line (RD)*, Laser Physics (2012) 22(2):477-478 (ISSN: 1054- 660X, I.F. 3.605) <https://doi.org/10.1134/S1054660X12020338>
15. N. Hassan, M. Irfan, N. A. Khan, S. Khan, A. Shakoor, A. Majid, and **S. Sikandar Hayat**, *Annealing effect on the excess conductivity of $Cu_{0.5}Tl_{0.25}M_{0.25}Ba_2Ca_2Cu_3O_{10-\delta}$ ($M=K, Na, Li, Tl$) superconductors*, Journal of Applied Physics (2012) 111(5):053914-053919 (ISSN: 0021-8979, I.F. 2.328) <https://doi.org/10.1063/1.3684601>
16. Hamida Fekirini, Boualem Serier, Farida Bouafia, Bel Abbes Bachir Bouiadjra, **S. Sikandar Hayat**, *Effect of precipitate-precipitate interaction on residual stress in welded structure*, Computational Material Science, (2012) 65:207-215 (ISSN: 0927-0256, I.F. 2.863)<http://dx.doi.org/10.1016/j.commatsci.2012.06.005>
17. F. Hussain, **S. Sikandar Hayat**, M. Imran, S. A. Ahmad, and Farida Bouafia, *Sintering and Coalescence of nanoparticles on Surfaces of Metals: A Molecular Dynamics Approach*, ComputationalMaterialScience, (2012)65:264-268(ISSN:0927-0256,I.F.2.863) <http://dx.doi.org/10.1016/j.commatsci.2012.07.033>
18. S. Souad, Boualem Serier, F. Bouafia, Bel Abbes Bachir Boudjra, **S. Sikandar Hayat**, *Analysis of the stresses intensity factor in alumina–Pyrex composites*, Computational Material Science, (2013)72:68-80; (ISSN: 0927-0256, I.F. 2.863) <http://dx.doi.org/10.1016/j.commatsci.2013.01.030>
19. S. Souad, Boualem Serier, F. Bouafia, Bel Abbes Bachir Boudjra, **S. Sikandar Hayat**, *Corrigendum to Analysis of the stresses intensity factor in alumina–Pyrex composites*, Computational Material Science, (2013) 74:165 (ISSN: 0927-0256, I.F. 2.863) <http://dx.doi.org/10.1016/j.commatsci.2013.03.038>
20. F. Hussain, **S. Sikandar Hayat**, Z. A. Shah, and S. A. Ahmad, *Effect of Crystal Defects on Melting Temperature of Ni and Al*, Chinese Journal of Physics (2013) 51(2):356-367 (ISSN: 0577-9073, I.F. 2.638) <http://dx.doi.org/10.6122/CJP.51.347>
21. F. Hussain, **S. Sikandar Hayat**, Z. A. Shah, N. Hassan and S. A. Ahmad, *Interaction of Point Defects with Twin-boundaries in Au: A Molecular Dynamics Approach*, Chinese Physics B (2013) 22(9):096102-096110 (ISSN 1674-1056, I.F. 1.469) <http://dx.doi.org/10.1088/1674-1056/22/9/096102>
22. Farida Bouafia, Boualem Serier, Nassim Serier, **S. Sikandar Hayat**, *Effect of Density and Pointed Corner Degree of Pore on Local Stress in Welded Structures: Defect in Marine Structures*, ISRN Mechanical Engineering, (2014) 2014: 1-7 (I.F.1.730) <http://dx.doi.org/10.1155/2014/834659>
23. G. Murtaza, Sibghat-Ullah, R. Khenata, A. H. Reshake, **S. Sikandar Hayat**, *Optoelectronic properties of $XYAs_2$ ($X=Zn, Cd$; $Y=Si, Sn$) chalcopyrite compounds*, Journal of optoelectronics and advanced materials (January- February 2014), Vol. 16, No. 1-2, p. 110-116 (I.F..56).
24. Sibghatullah, G. Murtaza, R. Khenata, A.H. Reshak, **S. Sikandar Hayat**, S. Bin Omran, *Towards from indirect to direct band gap and optical properties of XP_2 ($X=Zn, Cd$; $Y=Si, Ge, Sn$)*, Physica B. (2014) 441:94-99 (ISSN: 0921-4526, I.F.1.45).<http://dx.doi.org/10.1016/j.physb.2014.02.021>
25. Z. A. Shah, **S. Sikandar Hayat**, Z. Rehman, Farida Bouafia, *The molecular dynamic study of anharmonic effects at Cu(111) and Ag(111) surfaces in the presence of Cu-and Ag-trimer island*, Physics Letters A, 378 (2014)1727–1732 (I.F. 1.86).<http://dx.doi.org/10.1016/j.physleta.2014.04.018>
26. Z. A. Shah, **S. Sikandar Hayat**, Z. Rehman, S. S. Rahman and F. Bouafia, *Vacancy generation and adsorption of Cu atom at Ag(1 1 1) surface during diffusion of Cu-trimer*,

- Surface Review and Letters, Vol. 21, No. 5 (2014) 1450072-7 (ISSN:1739-6667, I.F. 0.734) <http://dx.doi.org/10.1142/S0218625X14500723>
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