PERSONAL INFORMATION

Saff E Awal Akhtar

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Sex: Female | Date of birth 21/01/2000 | Nationality | Pakistani

EDUCATION AND TRAINING

2020-present	**PHD. Solid State Physics**
Institution	University of the Punjab Lahore, Pakistan (www.pu.edu.pk)
2020-2022	**M.Phil. Solid State Physics**
Institution	University of the Punjab Lahore, Pakistan (www.pu.edu.pk)
CGPA	4.0 / 4.0
Thesis Title	Dft study to check the effect of exchange and correlation functionals on the electronic, magnetic, and thermoelectric properties of 1T-CrO_2.
Thesis Abstract	A comparative study for different exchange-correlation functionals LDA, PBE, and SCAN has been carried out for 2-dimensional 1T-CrO_2. It is a half-metallic ferromagnetic material with a 507K Curie temperature. We have computed the previous electronic results, DOS, and band structure by using SCAN. An ultra-wideband gap of 4.05 eV is noted in the spin-down channel that ensures 100 percent spin-polarized current over a wide range of temperatures. In the spin-up band structure, we observed a graphene-like behavior, a Dirac cone at a 'K' high symmetry point. For the thermoelectric properties of CrO_2, only SCAN has successfully described the correct physical trend of transport coefficients i.e. electrical conductivity, thermal conductivity, and Seebeck coefficient.

2016-2020	**Bachelor of Science in Physics (BS Hons)**
Institution	University of Gujrat, Gujrat, Pakistan (www.uog.edu.pk)
CGPA	3.60 / 4.0
Thesis Title	Periodic energy decomposition analysis of iodide adsorption on TM-doped-SiC slabs for application as counter electrode
Thesis Abstract	The exploration of platinum-free counter electrode (CE) materials is a hot area of research related to dye-sensitized solar cells. This work reports the potential of 3d and 4d transition-metal-doped SiC monolayers for use as CEs studied via periodic energy decomposition analysis. Adsorption of iodide was carried out to check the catalytic activity of the doped slabs, reactivity, energetics, and bonding properties of the doped slabs. The interaction energy was computed through Pauli, electrostatic, and orbital energy terms. Preparation energy, found using structurally and electrically unperturbed fragments, was examined in detail to reveal the relative value of the slabs. Comparative analysis revealed that Ti:SiC and Zr:SiC slabs have superior catalytic properties to a Pt slab.

2014-2016	**Higher Secondary School Certificate (Physics, Chemistry, Biology)**
Institution	Superior College for Girls, Main G.T. Road Gujranwala.
Marks	890 / 1100

2012-2014	**Secondary School Certificate (Physics, Chemistry, Biology)**
Institution	Seerat High School for Girls, Faiz e Alam Town, Gujranwala
Marks	921 / 1100

PUBLICATIONS

- Majid, A., Akhtar, S. E. A., Sandhu, Q. U. A., & Khan, M. I. (2021). Iodide Adsorption on Transition-Metal-Doped SiC Monolayers: A Density Functional Theory Based Bonding Analysis. J. Electron. Mater, 50(6), 3546-3556. (Impact Factor 2.047)
- Tariq, S., Saleem, M., Rao, J., Abdel-Latif, I. A., Mubarak, A. A., Bahir, A. A., ... & Ali, M. (2023). Pressure-induced effects on PrAO3 (A= Cr and Fe) ferromagnets: a DFT study for spintronic and energy storage devices. Chemical Papers. (Impact Factor 2.146)
- Nanosensors: Designing and Fabrication, Applications for Flexible Devices and Future Perspectives. Current Nanoscience -2021. (Impact Factor 1.513)
- Immobilization of enzymes on magnetic nanoparticles. International Journal of chem-informatics research. (2020)

RESEARCH INTERESTS

- Computational and theoretical condensed matter physics, 2d modelling.
- Theory and implementation of the different DFT methods.
- Electronic, Magnetic, Elastic, and Mechanical properties, thermoelectric coefficients.
- Phonon properties, electron-phonon coupling.

RELATED SKILLS

- **Modeling with Wien2k, ADF-BAND, BoltzTrap, and Quantum Espresso**
  Good experience in computational Material modeling using the above software under Density Functional Theory.
- **Linux- Ubuntu, Centose**
- **Origin, Xcrysden, Xmgrace, VESTA**
- **Latex, Microsoft word, Power point, Excel**
- **Mathematica, Matlab**
- Experience in field and lab work during my postgraduate and undergraduate research.

WORK EXPERIENCE

Designation	**Lecturer Physics**
Timeline	September 2023 - present
Organization	Women university Mardaan, Mardaan , KPK**.**

Designation	**Research Assistant**

Timeline	Dec 2022- August 2023
Organization	DFT lab, COE in solid state physics, University of the Punjab, Lahore
Designation	**HED College teacher intern (Physics)**
Timeline	Jan 2023-Jun 2023
Organization	Govt associate college for women, Thokar Niaz Baig, Lahore
Thesis Assisted	1. A DFT study of phonon properties and Reststrahlen band of Half-Heuslers Alloys MnCrX (X=As,Sb,P). 2. Elastic and mechanical properties of Half Heusler Alloys MnCrX (X=As, Sb, P): An Ab initio study 3. Elastic and mechanical properties of Half Heusler Alloys RuVX (X=As, Sb, P): An Ab initio study.

AWARDS

- Gold Medalist in M.Phil. Solid State Physics (2022), University of the Punjab, Lahore
- University Merit Scholarship for position holders (2020), University of Gujrat
- University Merit Scholarship for position holders (2019), University of Gujrat
- University Merit Scholarship for position holders (2018), University of Gujrat
- Achieved the Higher Education Commission of Pakistan award of the Laptop to the highest achiever in class (2018).

LANGUAGES

- English,
- Urdu (National language),
- Punjabi (Mother language)

REFERENCES

- Dr. Afaq Ahmad
  Professor
  Centre of Excellence in Solid State Physics
  University of the Punjab Lahore.
  Contact: +92 3454384289
  Email: aafaq.cssp@gmail.com

- Dr. Abdul Majid Sandhu
  Professor
  Chairperson of department
  Department of Physics
  University of Gujrat, Gujrat.
  Contact: +92 3328009610
  Email: abdulmajid40@gmail.com

- Dr. Muhammad Shahbaz
  Assistant Professor
  Department of Physics
  University of the Punjab Lahore.
  Contact: +92 3175482461
  Email: shahbaz.physics@gmail.com