SHAAN AMEER

RESEARCH

- I have strong experience of working with molecular dynamics and electronic structure codes based on density functional theory (DFT) including VASP, Quantum Espresso, and CASTEP. My research interests are:
- To compute electronic, optical, and magnetic properties of bulk and 2D layer/interfaces in condensed matter.
- To understand influence of defects like vacancies, anti-sites, and impurities on electronic, magnetic and optical properties of bulk, layer, and interfaces of condensed matter.
- To apply and develop formalism to compute behavior of quasi-particles in the novel quantum materials using first-principle approaches
- To incorporate machine learning methods to study the properties of novel materials.

Computational skills: Proficient in scientific programming using Python/C/C++ and working with high performance computing clusters

Languages: English, Hindi and Urdu

EXPERIENCE

Jan 2022–May 2022	Assistant Professor, Department of Physics, St Stephens College, University of Delhi, INDIA •Subjects taught: Mathematical physics (computation lab and theory), Elements of modern physics (lab), Waves and Optics (theory and lab)
Sep 2021–Jan 2022	Guest Faculty, Department of Physics and Astrophysics, University of Delhi, INDIA
EDUCATION	University of Delhi New Delhi, INDIA
February, 2021	Doctor of philosophy – Physics University of Delhi New Delhi, India <u>Specialization</u> : Density functional theory, electronic structure computations, reaction kinetics calculations, role of defects and impurity in influencing electronic properties of bismuth iron oxides: perovskite BiFeO ₃ and mullite Bi ₂ Fe ₄ O ₉ Ph.D. Supervisor: Prof. Vinay Gupta (Late)
July, 2013	Master of Science – Physics Department of Physics and Astrophysics, University of Delhi New Delhi, India First Division – College topper and University second position <u>Specialization</u> : Advanced solid-state physics, Quantum field theory and quantum electrodynamics, General theory of relativity and cosmology, Non-linear dynamics
July, 2011	Bachelor of Science – Physics Ramjas College, University of Delhi New Delhi, India First Division– College second topper Specialization: Physics (major), chemistry, and mathematics

Curriculum vitae

 Participated in the organization of the conference: International Symposium of integrated functionalities – 2017, held at Shangri-La Eros, New Delhi, India Volunteered in the 93rd, 94th, 95th, and 96th Annual Convocation of University of Delhi
•Awarded research fellowship on securing rank in the National Eligibility Test (NET) conducted at national level jointly by University Grants Commission and Council of Scientific and Industrial research, Government of India (2013-2015).
•Awarded Merit scholarship by Faculty of Science, University of Delhi (2012) given every year to the meritorious students in the first year of M.Sc. Physics.
 Awarded Best poster presentation at International Conference of Nanoscience and
Nanotechnology (ICNN-2013), Lucknow, India for the presentation on "MEMS based SnO ₂ gas sensor for the trace level detection of NO ₂ gas"
•Awarded college topper in M.Sc. Physics (2011-2013), University of Delhi, India.
•Secured second position in B.Sc. Physics (2008-2011), Ramjas College, New Delhi, India.

PUBLICATIONS Listed are my publications in peer-reviewed journals, and conference proceedings.

- 1. Ameer, S., Jindal, K., Tomar, M., Gupta, V., and Jha, P.K., 2021. Role of H impurity as compensating center in BiFeO₃ by first-principle calculations. *Physica Scripta*, 96, p. 125813.
- Ameer, S., Jindal, K., Tomar, M., Jha, P.K. and Gupta, V., 2020. Tunable electronic and magnetic properties of 3d transition metal doped Bi₂Fe₄O₉. *Journal of Magnetism and Magnetic Materials*, 509, p.166893.
- Ameer, S., Jindal, K., Tomar, M., Jha, P.K. and Gupta, V., 2020. The role of anunintentional carbon dopant in resolving the controversial conductivity aspects in BiFeO₃. *Physical Chemistry Chemical Physics*, 22(18), pp.1001010026.
- 4. Ameer, S., Jindal, K., Tomar, M., Jha, P.K. and Gupta, V., 2019. Insight into electronic, magnetic and optical properties of magnetically ordered Bi₂Fe₄O₉. *Journal of Magnetism and Magnetic Materials*, 475, pp.695-702.
- 5. Ameer, S., Jindal, K., Tomar, M., Kumar, A., Jha, P.K. and Gupta, V., 2018. A theoretical and experimental formalism of electronic structure of BFO: Cr thin films and modulation of their electrical properties upon visible light illumination. *Journal of Applied Physics*, 124(15), p.155304.
- 6. Ameer, S., Jindal, K., Sharma, S., Jha, P.K., Tomar, M. and Gupta, V., 2018. Structural, morphological and optical properties of BiFe_{0.99}Cr_{0.01}O₃ thin films. *Vacuum*, 158, pp.166-171.
- 7. Ameer, S., Tomar, M., Jha, P.K. and Gupta, V., 2018. Insight into the gas phase dissociation of CF₃CH₂I and its reactions with H and OH by first principles. *Journal of molecular modeling*, 24(11), pp.1-9.
- 8. Ameer, S., Jindal, K., Tomar, M., Jha, P.K. and Gupta, V., 2018. Effect of Li doping on the electronic and magnetic properties of BiFeO₃ by first principles. *Integrated Ferroelectrics*, 193(1), pp.123-128.

PRESENTATIONS/CONFERENCE-PROCEEDINGS

- Ameer, S., Jindal, K., Tomar, M., Jha, P.K. and Gupta, V., 2018, May. Study of half-metallicity in BiMn_xFe_{1-x}O₃. In AIP Conference Proceedings (Vol. 1953, No. 1, p. 110018). AIP Publishing LLC.
- 10. Ameer, S., Jindal, K., Tomar, M., Jha, P.K. and Gupta, V., 2018. Effect of Vacancies on Structural and Magnetic Properties of BiFeO₃. *Advanced Science, Engineering and Medicine, 10*(7-8), pp.741-744.
- 11. Ameer, S., Jindal, K., Tomar, M., Jha, P.K. and Gupta, V., 2021. Growth of highly oriented orthorhombic phase of Bi₂Fe₄O₉ thin films by pulsed laser deposition. *Materials Today: Proceedings* 47, p 1646.
- 12. Jindal, K., Ameer, S., Tomar, M., Jha, P.K. and Gupta, V., 2021. Influence of magnetic ordering on electronic, optical and magnetic properties of Bi2Fe4O9. *Materials Today: Proceedings* 47, p 1637.
- 13. "Growth and optimization of *Pbam* Bi₂Fe₄O₉ and *R3c* phase of BiFeO₃ by pulsed laser deposition", Shaan Ameer, Kajal Jindal, Monika Tomar, Pradip K. Jha, Vinay Gupta, oral talk presented at National conference on Recent Advances in Functional Materials held online during 5th-6th November 2020.

Curriculum vitae

- "Effect of H doping on structural and electronic properties of BiFeO₃ using first principles", Shaan Ameer, Kajal Jindal, Monika Tomar, Pradip K. Jha, Vinay Gupta, poster presentation at International Symposium on Functional Materials (ISFM-2018) held at Chandigarh, India during 13th -15th April 2018.
- 15. "Phase-pure highly oriented Bi₂Fe₄O₉ thin films grown using Pulsed laser deposition technique", Shaan Ameer, Kajal Jindal, Monika Tomar, Pradip K. Jha, Vinay Gupta, poster presentation at International Symposium on Functional Materials (ISFM-2018) held at Chandigarh, India during 13th -15th April 2018.
- 16. "Raman Spectroscopy and Photoluminescence study of Cr substituted BiFeO₃ thin films", Shaan Ameer, Kajal Jindal, Monika Tomar, Pradip K. Jha, Vinay Gupta, poster presentation at 6th International Symposium on Integrated Functionalities (ISIF 2017), held at Shangri-La Eros', NewDelhi, India during 10th -13th December, 2017.
- "Ab-initio studies of structural, magnetic and ferroelectric properties of La and Cr codoped BiFeO₃, Shaan Ameer, Kajal Jindal, Monika Tomar, Pradip K. Jha, Vinay Gupta, oral talk presented at 6th International Symposium on Integrated Functionalities (ISIF 2017), held at Shangri-La Eros', New Delhi, India during 10th -13th December, 2017.
- 18. "Ab-initio computations of optical properties of pristine BiFeO₃ using simplified LSDA+U functional", Shaan Ameer, Pradip K. Jha, Kajal Jindal, Monika Tomar, Vinay Gupta, oral talk presented at 10th National conference on Solid state chemistry and allied areas (ISCAS 2017), held at Delhi Technological University, New Delhi, India during 1st 3rdJuly, 2017.
- "Effect of Cr doping on dielectric properties of Bismuth Ferrite thin films", Shaan Ameer, Savita Sharma, Monika Tomar and Vinay Gupta, Poster Presentation at Asian Meeting on Ferroelectrics held at New Delhi during 7th-12th November, 2016.
- "Au/BiYFeO₃/ITO MMM structure for photovoltaic studies having potential solar energy harvesting applications", Shaan Ameer, Savita Sharma, Monika Tomar and Vinay Gupta, Oral presentation at International Conference on Advances in Nanomaterials and Nanotechnology held at Jamia Millia Islamia, New Delhi during 4th-6th November, 2016.
- 21. "A-site doped Bismuth Ferrite (Bi_{0.97}La_{0.03}FeO₃) thin film for photovoltaic applications", Shaan Ameer, Savita Sharma, Monika Tomar, Vinay Gupta, poster presentation at International Conference on Material Science and Technology held at New Delhi during 7th -10th March, 2016.
- 22. "MEMs based SnO₂ gas sensor for trace level detection of NO₂ gas", Anjali Sharma, **Shaan Ameer**, Avneet Singh, Reema Gupta, Lokesh Rana, Anil Arora, Monika Tomar and Vinay Gupta, poster presentation at International Conference on Nanoscience and Nanomaterials held at Lucknow during 18th -20th November 2013.