Curriculum Vitae

Aftab Alam
Associate Professor
Department of Physics
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Personal Profile

Date of Birth	18^{th} December, 1980
Sex	Male
Nationality	Indian (by Birth)
Marital Status	Married

Academic History

Post M. Sc.	Post M.Sc. course work from S. N. Bose Centre for Basic Sciences, Calcutta, India (The course work included written exams and oral presentations/seminars for credit evaluation).
M. Sc. (Master of Science)	Physics, Nuclear Physics (Specialization) University of Calcutta, India
B. Sc. (Bachelor of Science)	Physics (Honors), Mathematics and Chemistry University of Calcutta, India

Research Profile

Associate Professor	May 2017 - present
Assistant Professor	Aug 2013 - April 2017 Department of Physics IIT Bombay, Powai, Mumbai, INDIA
Research Staff	2010 - 2013
Area of Research	Structural, Magnetic and Quantum phase transition in intermetallic compounds Ames Laboratory, USA
Research Associate	2007 - 2010
Area of Research	Many body multiple-scattering electronic-structure calculation of complex alloys University of Illinois at Urbana Champaign, USA
Doctorate	2002 - 2007
Broad Area of Research	Computational Material Science
Thesis Title	Vibrational properties of disordered systems
Supervisor	Prof. Abhijit Mookerjee S. N. Bose National Centre for Basic Sciences, INDIA

Honors/Fellowship

- 2016: Invited for Editorial Board member of Advanced Materials Letters, Sweden
- 2016: International Association of Advanced Materials (IAAM) Scientist Medal for outstanding contribution in the field of *Advanced Materials Science and Technology* at European Advanced Materials Congress, Stockholm (Sweden)
- 2014: Selected for Young Scientist Award by DST.
- 2013: Selected for Young Faculty Award from IIT Bombay
- 2008: Selected in Marquis Who's Who in the World Biography.
- 2006: International Doctoral Fellowship at UIUC, Illinois, USA.
- 2002: Qualified the National Level Exam, National Eligibility Test (NET-CSIR) in Physics for a five year PhD fellowship, India.
- 2001: Qualified the National Level Exam, Joint Entrance Screening Test (JEST) in Physics for PhD fellowship, India.

Areas of Interest

- Develop advanced theory, algorithms and numerically efficient codes for many problem to predict and explain the properties, structure and behavior of materials.
- Recent interests involve (as part of new Materials Discovery proposal, Ames Lab.):
  - Structural, Magnetic and Quantum Phase Transition in Intermetallics.
  - Understanding exotic phases of Superconductors and Topological Insulators.
  - Effect of variable relaxation time on thermoelectric properties of materials
  - Electronic and Optical properties of solar harvesting materials
- Electronic Structure and Thermodynamics of Alloys :
  - Transition metals, Binary and Ternary Alloys.
  - Long-range, Partial and Short-Range Ordering in Alloys.
- Vibrational properties of intermetallic and disordered materials :
  - Phonon dispersion, vibrational entropy, short-range ordering.
- Response functions in materials with defects :
  - Electrical conductivity, Electronic and Lattice thermal conductivity

Experience and Skills

- Independently developed a generalised lattice dynamical method to study the phonon excitations in disordered alloys. Developed the associated code and made an interface with the widely used Plane-wave pseudopotential based Quantum-Espresso code. Applied to study the phonon dispersion, vibrational entropy, Inelastic neutron scattering cross-section and thermal transport properties in novel materials.
- Experienced with first-principles calculations to explore the electronic structure and thermodynamic properties of materials.
- Mastered many skills including TB-LMTO, KKR-CPA, VASP, Recursion Method and Tight-Binding Methods.
- Good at analytical derivation and proficient in FORTRAN programming.

Books

1. Book entitled *"Lattice Dynamics of disordered systems" by Aftab Alam,* published by Lambert Academic Publishing, Omniscriptum GmbH & Co. KG, Bahnhoftrase 28, 66111, Saarbruken Deutschland/Germany

Complete list of papers published/under review in Scientific Journals

After Joining IIT Bombay (Accepted/Under Review)

1. Jiban Kangsabanik, R. K. Chouhan and **Aftab Alam**, *Effect of random correlations on lattice dynamical properties of disorder* $Au_{1-x}Fe_x$ *alloys* (*Under Review, 2017*)
2. C. K. Barman, Prashant Singh, D. D. Johnson and **Aftab Alam**, *Hidden and coexistent low temperature magnetic phases in Kondo type Cerium Hexaboride*, (*Under Review, 2016*)

After Joining IIT Bombay (Published)

1. Vikram, Jiban Kangsabanik, Enamullah and **Aftab Alam**, *Bismuth based Half Heusler Alloys with giant thermoelectric figure of merit, J. Mater. Chem. A* **5**, 6131-6139 (2017).

2. Jiban Kangsabanik, Vikram and **Aftab Alam**, *La-doped* $CH_3NH_3BaI_3$ *: A promising transparent conductor, Adv. Mater. Lett.* **8(4)**, 002-007 (2017).

3. Akash Kumar, K. R. Balasubramaniam, Jiban Kangsabanik, Vikram, and **Aftab Alam**, *Crystal structure, stability and optoelectronic properties of the organic-inorganic wide-band-gap perovskite* $CH_3NH_3BaI_3$*: Candidate for transparent conductor applications Phys. Rev. B* **94**, 180105 (R) (2016).

4. Enamullah, D. D. Johnson, K. G. Suresh and **Aftab Alam**, *Half-metallic, Co-based quaternary Heuslers for spintronics: defect- and pressure-induced transitions and properties*, *Phys. Rev. B* **94**, 184102 (2016).

5. Enamullah, Y. Venkateswara, Sachin Gupta, Manoj Raama Varma, Prashant Singh, K. G. Suresh and **Aftab Alam**, *Electronic structure, magnetism and antisite disorder in CoFeCrGe and CoMnCrAl Alloys*, *Phys. Rev. B* **92**, 224413 (2015).

6. Lakhan Bainsla, A. I. Mallick, **Aftab Alam**, K. G. Suresh *et al.*, *Origin of spin gapless semiconductor behavior in CoFeCrGa : Theory and Experiment*, *Phys. Rev. B* **92**, 045201 (2015).

7. Lakhan Bainsla, A. I. Mallick, **Aftab Alam**, K. G. Suresh *et al.*, *High spin polarization and large spin splitting in equiatomic quaternary CoFeCrAl Heusler Alloy* , *J. Magn. and Magnetic Mater.* **394**, 82-86 (2015).

8. Lakhan Bainsla, A. I. Mallick, M. Manivel Raja, A. K. Nigam, B. S. D. Ch. S. Varaprasad, Y. K. Takahashi, **Aftab Alam**, K. G. Suresh, and K. Hono, *Spin gapless semiconducting behavior in equiatomic quaternary CoFeMnSi Heusler alloy*, *Phys. Rev. B* **91**, 104408 (2015).

9. **Aftab Alam**, Suffian N Khan, A. V. Smirnov, D. M. Nicholson and Duane D. Johnson, *Greens function multiple-scattering theory with a truncated basis set: An Augmented -KKR formalism*, *Phys. Rev. B* **90**, 205102 (2014).

10. D. D. Johnson, **Aftab Alam**, A. Pathak, V. Pecharsky, K. Gschneidner Jr., R.W. McCallum, *Better (Non) Rare-Earth Magnets - Using DFT Methods as a Computational Design Tool for Replacing Critical Materials*, *Proceedings : 23rd International Workshop on Rare-Earth and Future Permanent Magnets and Their Applications (REPM-2014), G.C. Hadjipanayis, C. H. Chen, J.P. Liu, editors, pp. 450-453, Annapolis, Maryland, USA (August 17-21, 2014)*

11. **Aftab Alam** and D. D. Johnson, *Mixed valency and site-preference chemistry for Cerium and its compounds : A predictive DFT study*, *Phys. Rev. B* **89**, 235126 (2014).

12. S N Khan, **Aftab Alam** and D D Johnson, *Fermi surface and phase stability of Ba(Fe,M)$_2$As$_2$ with (M=Co, Ni,Cu, Zn)*, *Phys. Rev. B* **89**, 205121 (2014).

13. R. K. Chouhan, **Aftab Alam**, S. Ghosh and A Mookerjee, *Interplay of force constants in the lattice dynamics of disordered alloys: An ab-initio study*, *Phys. Rev. B (Rapid Commun)* **89**, 060201(R) (2014).

14. S N Khan, **Aftab Alam** and D D Johnson, *Low-energy, planar magnetic defects in BaFe$_2$As$_2$: nanotwins, twins, antiphase and domain boundaries*, *Phys. Rev. B* **88**, 184515 (2013).

Before Joining IIT Bombay (Published)

1. L. L. Wang, **Aftab Alam** *et al.*, *Native Defects in Tetradymite Bi$_2$(Te$_x$Se$_{3-x}$) Topological Insulators*, *Phys. Rev. B* **87**, 125303 (2013).
2. **Aftab Alam**, M Khan, R W McCallum and D. D. Johnson, *Site-preference and valency for rare-earth sites in (R-Ce)$_2$Fe$_{14}$B magnets*, *Appl. Phys. Lett.* **102**, 042402 (2013).
3. M. G. Kim, **Aftab Alam** *et al.*, *Effects of transition metal substitutions on the incommensurability and spin fluctuations in BaFe$_2$As$_2$ by elastic and inelastic neutron scattering*, *Phys. Rev. Lett.* **109**, 167003 (2012).
4. **Aftab Alam**, B.G. Wilson and D. D. Johnson, Reply to Comment on *"Accurate and Fast numerical solution of Poisson's equation for arbitrary, space-filling Voronoi polyhedra: near-field corrections revisited "*, *Phys. Rev. B* **86**, 127102 (2012).
5. **Aftab Alam**, Biplab Sanyal and A. Mookerjee, *Effect of disorder on the electronic properties of graphene: A theoretical approach*, *Phys. Rev. B* **86**, 085454 (2012).
6. Rajiv K. Chouhan, **Aftab Alam**, Subhradip Ghosh and Abhijit Mookerjee, *Ab-initio study of the phonon spectrum, entropy and lattice heat capacity of disordered Re-W alloys*, *J. Phys. : Condens Matter* **24**, 375401 (2012).
7. **Aftab Alam** and D. D. Johnson, *Structure and Relative Stability of (Meta)Stable Ordered, Partially-ordered and Disordered Al-Li Alloy Phases*, *Phys. Rev. B* **85**, 144202 (2012).
8. **Aftab Alam**, Rajiv K Chouhan and Abhijit Mookerjee, *Thermal conductivity and diffusion-mediated localization in Fe$_{1-x}$Cr$_x$ Alloys* from first principles, *Phys. Rev. B* **84**, 224309 (2011).
9. **Aftab Alam**, B.G. Wilson and D. D. Johnson, *Accurate and Fast numerical solution of Poisson's equation for arbitrary, space-filling Voronoi polyhedra: near-field corrections revisited*, *Phys. Rev. B* **84**, 205106 (2011).
10. **Aftab Alam** and D. D. Johnson, *Chemically-Mediated Quantum Criticality in NbFe$_2$*, *Phys. Rev. Lett.* **107**, 206401 (2011).

11. **Aftab Alam**, S.N. Khan, B.G. Wilson and D. D. Johnson, *Efficient integration over Complex Voronoi Polyhedra for Electronic Structure Calculations*, *Phys. Rev. B* **84**, 045105 (2011).
12. B.G. Wilson, D.D. Johnson, and **Aftab Alam**, *Multi-center electronic structure calculations for plasma equation of state*, *High Energy Dens. Phy.* **7**, 61-70 (2011).
13. **Aftab Alam**, Rajiv Kumar Chouhan and Abhijit Mookerjee, *Vibrational Entropy of Fe-Cr alloy with short-range order: A first-principles calculation*, *Phys. Rev. B* **83**, 054201 (2011).
14. **Aftab Alam**, Brent Kraczek and D. D. Johnson, *Structural, Magnetic and Defect Properties of Co-Pt-type Magnetic-Storage Alloys: density-functional theory study of thermal processing effects*, *Phys. Rev. B* **82**, 024435 (2010).
    *Chosen as focused article of frontier research in **Virtual journal of nanoscale Science & Technology**, Vol. 22, Issue 7 (2010).
15. **Aftab Alam** and Abhijit Mookerjee, *Ab-initio electronic structure of disorder ternary alloys : A reciprocal space formulation*, *Phys. Rev. B* **81**, 184205 (2010).
16. **Aftab Alam**, T. Saha-Dasgupta and Abhijit Mookerjee, *Ab-initio augmented space recursion to study complex multicomponent materials: Application to the pseudo-binary alloy* $Ni_{1-x}Pt_xAl$, *Phys. Rev. B* **81**, 054201 (2010).
17. **Aftab Alam** and D. D. Johnson, *Optimal site-centered electronic-structure basis set from a displaced-center expansion: Improved results via* a priori *estimates of saddle-points in the density*, *Phys. Rev. B* **80**, 125123 (2009).
18. **Aftab Alam** and Abhijit Mookerjee, *An augmented space approach to the study of random ternary alloys: I. Electronic structure with uncorrelated disorder and short range ordering*, *J. Phys. : Condens Matter* **21**, 195503 (2009).
19. **Aftab Alam**, T. Saha-Dasgupta, A. Mookerjee, A. Chakrabarty and G.P. Das, *Electronic structure and phase stability of disordered hexagonal closed packed alloys* , *Phys. Rev. B* **75**, 134203 (2007).
20. **Aftab Alam**, Subhradip Ghosh and Abhijit Mookerjee, *Phonons in disordered alloys : Comparison between augmented-space-based approximations for configuration averaging to integration from first principles*, *Phys. Rev. B* **75**, 134202 (2007).
21. **Aftab Alam** and A Mookerjee, *Lattice thermal conductivity of disordered NiPd and NiPt alloys : A numerical study*, *J. Phys.: Condens Matter* **18**, 4589 (2006)
22. Kartick Tarafder, Kamal K. Saha, **Aftab Alam** and Abhijit Mookerjee, *Response functions in disordered alloys : an approach via the augmented space recursion.*, *Journal of Physics : conference series* **29**, 27 (2006).
23. **Aftab Alam** and Abhijit Mookerjee, *Inelastic neutron scattering in random alloys*, *Proceedings of the DAE Solid State Physics Symposium* Vol. **50** 679-680 (2005).
24. **Aftab Alam** and Abhijit Mookerjee, *Lattice thermal conductivity of disordered binary alloys*, *Phys. Rev. B* **72**, 214207 (2005).
25. **Aftab Alam** and Abhijit Mookerjee, *Inelastic neutron scattering in random binary alloys : An augmented space approach*, *Phys. Rev. B* **71**, 094210 (2005).
26. **Aftab Alam** and Abhijit Mookerjee, *Phonons in disordered alloys*, *Proceedings of the DAE Solid State Physics Symposium* Vol. **49** 590-591 (2004).
27. **Aftab Alam** and Abhijit Mookerjee, *Vibrational properties of phonons in random binary alloys : An augmented space recursive technique in k-space representation*, *Phys. Rev. B* **69**, 024205 (2004).

Work in progress (various collaborations)

1. Search for Cerium-based permanent magnets: under ARPA-E project (in collaboration with *R W McCallum* (experimentalist) of Ames Laboratory, USA)
2. Electronic transport in dense plasmas via Greens function approach: under HEDP project (in collaboration with *B G Wilson* of Lawrence Livermore Natl. Lab, USA)
3. Investigating surface band properties of simple intermetallic compounds with dirac-cone like bands (in collaboration with *Liqin Ke* of Ames Laboratory, USA)
4. Electronic properties and Dirac-cone fermiology of disordered Graphene: (in collaboration with *Biplab Sanyal* of Uppsala University, Sweden)
5. Vibrational properties of intermetallic alloys: An *ab-initio study* (in collaboration with *R K Chouhan*, Boise State University, Idaho, USA)
6. Investigating more optimized exchange correlation functionals for band gaped materials (in collaboration with *Prashant Singh* of Ames Laboratory, USA)
7. Electronic Structure of newly emerging spin gapless semiconductors (in collaboration with K G Suresh (experimentalist) of Physics department, IIT Bombay)
8. First principles study of thermoelectric materials (in collaboration with Titas Dasgupta of Materials Science & Engineering department, IIT Bombay)

Teaching at IIT Bombay

1. Quantum Physics & Application (PH-107), Autumn 2016:Students Feedback - 80%
2. Theor. Condens. Matt. Physics (PH-522), Spring 2016 : Students Feedback - 91%
3. Quantum Physics & Application (PH-107), Autumn 2015:Students Feedback - 71%
4. Theor. Condens. Matt. Physics (PH-522), Spring 2015 : Students Feedback - 99%
5. Mathematical Physics I (PH-407), Autumn 2014 : Students Feedback - 77%
6. Theor. Condens. Matt. Physics (PH5-22), Spring 2014 : Students Feedback - 94%

Invited Talks

1. TPSC talk on *First principles thermodynamic calculation of hcp disordered alloys* , **Indian Institute of Technology**, Roorkee, INDIA ; 13th November 2006.
2. TPSC talk on *Electronic structure and Phase stability of disordered hcp alloys* , **Indian Institute of Technology**, Guwahati, INDIA ; 25th September 2006.
3. *Vibrational and thermal properties of disordered alloys : A theoretical study* , **16-th Symposium on thermo physical properties**, NIST Boulder, Colorado, USA ; 30 July - 04 August 2006.
4. *Disorder-mediated quantum criticality in Laves phase* $NbFe_2$, **Condensed Matter Physics Lunch Talk**, Ames Laboratory; 31st January 2012.
5. *Low-energy magnetic defects at nano- and meso-scale in Fe-based superconductors* , **Structural and Physical Properties of Solids**,Indian School of Mines, Dhanbad; 19th November 2013.
6. *Interplay of force constants and short-range ordering in the lattice dynamics of disordered alloys*, **Asia Sweden meeting on understanding functional materials from lattice dynamics**, IIT Guwahati; 10th January 2014.
7. Attended a meeting on **Strongly Correlated Systems: from Models to Materials**, Indian Institute of Science, Bangalore; 11 - 13th January 2014.

8. *Magnetic planar and point defects in Pnictide superconductors*, **International Conference on Electrical, Electronics, Engineering Trends and Sciences**, Dhanekula Engineering College, Hyderabad; 12th October 2014.

9. *Pressure and disorder mediated transitions in quaternary Heusler alloys : An ab-initio study,* **Functional materials for today and tomorrow, Hotel Hindustan International, Kolkata; 28-30 October 2015.**

10. *Bismuth based half-Heusler alloys with giant thermoelectric figure of merit,* **DAE Solid State Physics Symposium, KIIT Bhubhaneswar; 26-30 December 2016.**

Selected list of visits, presented talks/posters

1. *Accurate solution of Poisson equation for arbitrarily shaped space filling Voronoi polyhedra*, **APS March Meeting 2012**, Boston, Massachusetts, USA ; 27 Feb to 2 March 2012.

2. *Disorder-induced quantum criticality in* $NbFe_2$, **APS March Meeting 2011**, Dallas, Texas, USA ; 21-25 March 2011.

3. *Structural defect properties of CoPt-type magnetic storage alloys*, **APS March Meeting 2010**, Portland, Oregon, USA ; 15-19 March 2010.

4. *Optimized basis-set representation for electronic-structure methods: Better Energetics* , **APS March Meeting 2009**, Pittsburgh, Pennsylvania, USA ; 16-20 March 2009.

5. Project on *sp3-hybrid orbitals for tetrahedrally bonded semiconductors* with Prof. O. K. Andersen during a month visit at the **Max. Planck Institute, Stuttgart, Germany**; May-June 2006.

6. *Thermal transport properties of* $Ni_{1-x}T_x$ *(T=Pd,Pt) alloys* at the **INDO-US Conference on novel and complex materials**, S N Bose National Centre (SNBNCBS), Kolkata, India; 26-29 October 2005.

7. Paper entitled *Vibrational properties of random binary alloys : An augmented space recursive technique in the k-space representation* , **In-House meeting 2003**, SNBNCBS, Kolkata, India; 27-29 January 2004.

8. *Phonons in disordered alloys* , **Workshop and Conference on physics of novel materials**, SNBNCBS, Kolkata, India; January 5-14, 2004.

9. Poster on *Lattice thermal conductivity of disordered binary alloys* , in the **50th DAE solid state physics symposium**, Bhabha Atomic Research Centre and TIFR, Mumbai, India; December 5-9, 2005.

10. Project on *Solving the spinless Falicov Kimball model within the Hartree Fock approximation* , in the **SERC school on strongly-correlated electron systems**, Harish Chandra research institute, Allahabad, India; November 15-27, 2004.

Sponsored projects/Proposals

1. (In USA) Co Principal Investigator of (Ames Lab. + LLNL) joint proposal entitled: *" Electronic Transport in Dense Plasmas via Multicenter Greens Function Techniques "* (April 2012 -) ; $100 K. This eventually facilitated the remote access to their giant High Performance Computing Cluster even after joining IIT Bombay (till date).

2. (In India) Principal Investigator of IRCC SEED grant proposal entitled:
   " Spherical to Full Potential based Ab-initio Density Functional Method : Application to Newly Emerging Materials " (January 2014 -) ; INR 20 Lakhs

3. (In India) Principal Investigator of DST (SERB) project entitled:
   " Electronic Structure, Phonons and Transport properties of Disordered Graphene "
   (October 2014 -) ; INR 17 Lakhs

4. (In India) Co Principal Investigator of National Centre for Photovoltaic Research & Education (NCPRE) Proposal, funded by Ministry of New and Renewable Energy (2016 to 2021); INR 45 Lakhs

5. (In India) Co Principal Investigator of Indo(DST)-Korea joint proposal entitled:
   "Development of Cheap/Efficient Flexible Perovskite Solar Cells for Portable Power Supply"
   INR 35 Lakhs (Under review)

Other Services/Experience/Achievements

1. **Referee :**
   Physical Review Lett., Phys. Rev. B, Appl. Phy. Lett., J. Appl. Phys., Comp. Phys. Commun., Mod. Phys. Lett. B, IJMPB, J. Phys.: Cond. Matt., IEEE
2. **Mentored 2 PhD. students (during the tenure in USA) :**
   1) S N Khan, University of Illinois, Urbana Champaign, USA (now post-doc at Oak-Ridge Natl. Lab, USA)
   2) R K Chouhan, SNBNCBS, India (now post-doc at Boise State University, USA)
3. Organized a symposium (SYMPHY) in physics, IIT Bombay, April 2015
4. Served as a General Secretary of Iowa State University Post-Doctoral Association (ISUPDA), USA, 2012 - 2013
5. Member of American Physical Society (APS).
6. Editorial of Advanced Materials Letter (AML).

Research Group

1. **Aftab Alam (Group Leader)**

2. Dr. Enamullah Khan, Post-doc Fellow (prior position : IIT Guwahati)
3. Arif Iqbal Mallick, PhD. (prior position : IIT Madras)
4. Arindam Sarkar, PhD. (prior position : Bengal Engg. & Science Univ, Kolkata)
5. Vikram, PhD. (prior position : IIT Bombay)
6. Jiban Kangshabanik, PhD. (prior position : IIT Bombay)
7. Chanchal K. Barman, PhD. (prior position : IISc. Bangalore)
8. Deepika Dabra, PhD. (prior position : University of Delhi) ; as Co-Guide

Complete Addresses of the referees

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