Dr. Dibya Prakash Rai

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Present Address
Department of Physics
Pachhunga University College
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Sivitar T. E
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India-734203

Ph.D. Dissertation:

I have studied the electronic and magnetic properties of transition metal based Heusler compounds by using the density functional theory (DFT). A DFT relies upon the Kohn-Sham (KS) equation with inclusion of exchange-correlation potential to improve the accuracy. The most commonly used exchange-correlation functional are generalized gradient approximation (GGA-PBE, Perdew, Burke and Ernzerhof), local (spin) density approximation LDA/LSDA, modified Becke Johnson (mBJ) potential, etc. Magnetic properties are natural outputs of the calculations and itinerant magnetism can be discussed in a more qualitatively. The more relevant method LSDA+U (Coulomb repulsion) formalism is used to treat the strongly correlated electrons for better accuracy of the ground state properties. A code Wien2k based on full potential linearized augmented plane wave (FP-LAPW) method within DFT is adopted. We mainly focus on the half-metallicity (HMF) of $L2_1$ type full Heusler alloys with formula X_2YZ (X,Y = Sc, Ti, V, Mn, Fe, Co and Z = Al, Si, Ga, Ge, As, etc).

Education

July 2013-Dec 2014: Post Doctoral Fellow (PDF) in the group of Prof. San-Huang Ke, Beijing Computational Science Research Center, Beijing 100084, Peoples Republic of China.
2009-2013: Ph.D. under the supervision of Prof. R. K. Thapa, Mizoram University, Mizoram, Aizawl, India.
2007-2009: M.Sc., Mizoram University, Mizoram, Aizawl-796004, India.
2002-2005: B.Sc. St. Joseph's College (North Point) Darjeeling, India.
Ph.D Thesis Title: *Study of electronic and magnetic properties of half metallic transition metal based Heusler compounds*

Experience

Assistant Professor	Department of Physics, Pachhuncga University College	16 Dec 2014-Present
Postdoctoral Fellow	Computational Science Research Center Beijing, China	(2013-2014)
Assistant Teacher	Delhi Public School, Siliguri, India	2006-2007 (1.6 years)

Research Interest

1. Transition Metal based strongly correlated materials (Heusler compounds, half metals).
2. Semiconductors, insulators, semi-metals.
3. Thermoelectric materials and their properties (focusing on their efficiency).
4. Theoretical techniques (doping of heavy elements, 2D single/multi atomic layers, superlattices, nanostructuring) are implimentated to see the effect of the band energies near Fermi level.
5. Employing first principles method (Density Functional Theory, DFT) for calculation.

Current Projects

1.**Project Title :** A first principles study of perovskite compounds, a probe for solar cell materials.
Sponsor: UGC-BSR,FRPS, Start-Up Grant Lett.No.F.30-52/2014(BSR)(*on going*)
Budget: Rs.6,00,000.

Computer Skills

1. Extensive knowledge of hardware and software (can use DOS, Windos, LINUX)
2. Elementary programming skills in FORTRAN and C++.
3. Proficient in using software packages WIEN2K (DFT, code) and Exciting, Octopus (DFT/TD-DFT, code)
4. Basic knowledge in using KKR (a code based on multiple scattering theory, Green function technique).
5. Can use Cluster-Computer (16-nodes), parallel computation, FTP.
6. Efficient in Latex, Origin, Gnuplot, Xmgrace, Excel.

Journal Reviewed

1. **Elsevier:** Journal of Alloys and Compounds, Physica B, Physics and Chemistry of Solids, Materials Science and Semiconductor Processing, Journal of Magnetism and Magnetic Materials, Intermetallics
2. **Taylor & Francis:**Phase Transition, Complex Metals
3. **Open Access Library:** Chinese Journal
4. Journal of Advances in Physics.
5. **Columbian Journal:**Engineering and Science Journal.
6. **World Scientific:** International Journal of Modern Physics B, International Journal of Modern Physics C, Journal of Theoretical and Computational Chemistry.
7. **Springer:** Indian Journal of Physics, Journal of Electronic Materials.
8. **Turkish Journal:**Zeitschrift fr Naturforschung A:-A Journal of Physical Sciences.
9. **International Knowledge Press:** Journal of Applied Physical Science International.
10. **RSC:** Advances.

Project Reviewed:

Czech Science Foundation (Czech Republic): Material preparation and metallurgy.

Honors and Awards

1. Received Nehru Award for the meritorious students of the ward of Tea Plantation workers (2000).
2. MSc. in Physics, first class first, Gold medalist (2009).
3. Received INSPIRE-DST Research Fellowship (Department of Science & Technology, Govt. of India, New Delhi) 2009-2012, Ph.D.
4. Best oral presentation in 8th National Conference on Physics Academy of North East India, Department of Physics, Mizoram University, Aizawl. 17-19 December, 2012
5. Editorial board member of Wudpecker Journal of Educational Research.
6. Reviewer of Public Journal of Physical Science.
7. International Scientific and Technical Committee & Editorial Review Board Member of World Academy of Science, Engineering and Technology, USA.
8. Executive council member of Indian Nano Biologist Association (INBA), Madurai, Tamil Nadu (Aizawl Chapter).
9. Editorial board member of International Journal of Modern Chemistry and Applied Science (IJMCAS), ISSN:2349-0594.
10. International Scientific Committee and Editorial Board member of Physical and Mathematical Sciences (International Science Index).
11. Editorial board member of International Journal of Applied Research (IJAR), P-ISSN Number: 2394-7500.
12 Editorial board member of International Journal of Advancement in Engineering Technology, Management & Applied Science (IJAETMAS).
13.Editorial board member of International Journal of Engineering Research Science (IJOER), ISSN No.2395-6992.
14. Editorial board member of SSRG International Journal of Applied Physics (SSRG-IJAP), ISSN: 2350-0301.
15. Editor of the International Journal of Research in Medical and Basic Sciences (IJRMS).
15. Advisory/Editorial board member of nternational Journal of Innovative Research in Engineering Management (IJIREM), India, ISSN:2350-0557.

16. Editorial board member of International Journal of Physics and Applications (IJPA), Research India Publications.
17. Editorial board member of International Journal of Current Research in Chemistry and Pharmaceutical Sciences (IJCRCPS).
18. Editorial board member of World Journal of Nano Science and Engineering, Scientific Research: an Academic Publisher (Open Access).
19. Editorial Manager of Journal of material Science, Research & Review international journals ISSN: 2321-6212 (Open Access).
20. Editorial board member of Journal of Materials Science and Surface Engineering (JMSSE), ISSN(Online): 2348-8956.
21. Editorial board member of International Journal of Physics and Research (IJPR), Transstellar Journal Publications and Research, ISSN(Print): 2250-0030.
22. Editorial board member of International Journal of Recent Technology and Engineering(IJRT), Exploring Innovation, ISSN:2277-3878(Online).
23. Editorial board member of American Journal of Applied Sciences, Engineering and Technology (AJASET), Science Publishing Group.
24. Academic Editor of Physical Science International Journal, SCIENCEDOMAIN international, ISSN:2348-0130.
25. Editorial board member of Advanced Science and Technology Journal(http://s.astjournal.com/index.php/ast).
26 Editorial board member of International Journal of Material Science (IJMSCI),Science and Engineering Publishing Company, ISSN:2226-4531.
27. Editorial board member of Advances in Materials Science and Engineering: An International Journal (MSEJ),AIRCC Publishing Corporation, ISSN:2394-0824.
28. Editorial board member of International Journal of Innovative Science and Modern Engineering (IJISME),ISSN:23196386.
29. Guest Editor of International Journal of Materials Science and Applications / Energy and Materials, ISSN Print:2327-2635.
30. Associate Editor of Journal of Chemical, Biological and Physical Sciences (JCBPSC), ISSN:2249-1929.

Life membership

1. Life member (LM-0169) of Physics Academy of North East India (PANE), Gauhati.
2. Life member (LM-1058) of Indian Physical Society, IACS, Kolkata.
3. Life member (LM-13090) of Indian Physics Association, BARC, Mumbai.
4. Life member (LM-B2406) of Material Research Society of India, IISc, Banglore.
5. Life member (L-697) of Optical Society of India, Calcutta University, Kolkata.
6. Life member (L6773) of Indian Association of Physics Teachers (IAPT), IIT, Kanpur.
7. Life member (LM-388) of Indian Association of Solid State Chemists and Allied Scientists (ISCAS), Jammu University, Jammu.
8. Life member (LM-664) of Magnetic Society of India (MSI), Defence Metallurgical Research Laboratory, Hyderabad.
9. Life member (LM-611) of Indian Crystallographic Association (ICA), IISc. Bangalore.
10. Life member (LM-2120) of Solar Energy Society of India(SESI), New Delhi.
11. Life member (LM-1378) of Punjab Academy of Sciences(PAS), Punjab University, Patiala.
12. Life member (LM-1082) of Indian Institute of Mineral Engineers(IIME), Jamshedpur.
13. Life member (LM-R32) of Indian Society for Surface Science and Technology (ISSST), Jadavpur University, Kolkata.
14. Life member (L26686) of Indian Science Congress Association, Kolkata.
15. Life member (LM-5576) of Assam Science Society (ASS), Guwahati, Assam.
16. Life member (LM-103240) of Indian Society for Technical Education, IIT Delhi Campus, New Delhi.
17. Life member (LM-869) of Society for Material Chemistry (SMC), Bhabha Atomic Research Centre, Mumbai.
18. Life member (LM-1627) of Indian society for Advancement of materials and Processing (ISAMPE), Aeronautical Society of India Building, New Thippasandra, Bangalore-560075.
19. Life member of Indian Nano Biologists Association (INBA), Madurai, Tamil Nadu.

20. Life member (201506678) of Semiconductor Society of India (SSI) University of Delhi South Campus, New Delhi-110021, India.

Publications in National/International journals

2010

1. **D. P. Rai**, D. T.Khating , P. K.Patra , J. Hashemifar, M. Jamal, Lalmuanpuia, M. P. Ghimire, Sandeep, Rosangliana and R. K. Thapa "Study of Co_2MnAl Heusler alloy as half-metallic ferromagnet" *Indian Jour. Phys.* 84 (5) (2010) 593-59. [ISSN:0973-1458, IF:1.785]

2011

2. **D. P. Rai**, M. P. Ghimire and R. K. Thapa "Study of energy bands and magnetic properties of Co_2CrSi Heusler Alloy" *Bull. Mat. Sc.* 34 (2011) 1219-1222. [ISSN: 0250-4707, IF:0.88]

2012

3. Sandeep, **D. P. Rai**, M. P. Ghimire, J. Maibam and R. K. Thapa "First principle calculations of the electronic and magnetic properties of semi-Heusler alloys like NiVSb and NiTbSb" *Indian Jour. Phys.* 86 (2012) 301-305 [ISSN:0973-1458, IF:1.785]

4. **D. P. Rai** and Thapa R. K. "Electronic Structure and Magnetic Properties of X_2YZ (X=Co, Y=Mn, Z=Ge, Sn) type Heusler Compounds : A first Principle Study" *Phase transition: A multinational Jornal* 85(7) (2012) 1-11.[ISSN: 0141-1594, IF=1.006]

5. **D. P. Rai**, A. Shankar, Sandeep, M.P. Ghimire and R.K. Thapa, Electronic and magnetic properties of X_2YZ (X= Co, Y = Cr, Z=Al, Ga) Heusler compounds: A First Principles method *Int. Jour. Mord. Phys. B* 26, 8 (2012) 1250071. [ISSN: 0217-9792, IF=0.558]

6. **D. P. Rai**, A. Shankar, Sandeep, M. P. Ghimire and R. K. Thapa, "A Ground state Study of Structural and magnetic properties of Co_2CrGe: A GGA method" *Materials Research India* 9(1). 155-158 (2012). [ISSN: 0973-3469]

7. **D. P. Rai**, A. Shankar, Sandeep, M. P. Ghimire and R. K. Thapa, "A comparative study of a Heusler alloy Co_2FeGe using LSDA and LSDA+U" *Physica B* 18 (2012) 3689-3693. [ISSN: 0921-4526, IF=1.135]

8. **D. P. Rai**, A. Shankar, Sandeep, M. P. Ghimire and R. K. Thapa, "A First Principles study of Co_2MnSi a full-Heusler compound: LSDA Method" *Int. Jour. Comp. Phys. Sci.* 3 (2012) 21-27. [ISSN: 0976-5875]

9. **D P Rai**, Sandeep, A Shankar, M P Ghimire and R K Thapa, "Ground State Study Co_2VAl: LSDA+U method" *Physica Scripta* 86 (2012) PS422049.[ISSN: 1402-4896, IF=1.032]

10. **D. P. Rai**, A. Shankar, Sandeep, M.P. Ghimire and R.K. Thapa, " Electronic structure and magnetic properties of Co_2MnSi by using LSDA+U method" *Asian Jour. of Phys. Sci.* 1(1) (2012) 10-25. [ISSN:2186-8492]

11. **D. P. Rai** and R.K. Thapa "A density functional theory (DFT) study of Co_2CrGe: LSDA method" *Lat. Am. J. Phys. Educ.* 6 (2) (June 2012) 317-321. [ISSN:1870-9095]

12. **D. P. Rai**, A. Shankar, Sandeep, M.P. Ghimire and R. K. Thapa "Study of Half-metallic properties in Co_2CrSb using GGA and LSDA" *Int. J. Phys. Maths. Sci.* 2 (2012) 46-69. [ISSN: 2010-1791]

13. **D. P. Rai**, A. Shankar, Sandeep, Rosangliana and R. K. Thapa "Study of the structural properties of Co_2YGe (Y=Sc, Ti, V, Cr, Mn, Fe) by GGA method" *Science Vision* 12 (2012) 74-78. [ISSN: 0975-6175]

14. **D. P. Rai** and R.K. Thapa, "An investigation of semiconducting behaviour in the minority spin of Co_2CrZ (Z = Ga, Ge, As): LSDA and LSDA+U method" *Journal of Alloys and Compounds* 542 (2012) 257263. [ISSN: 0925-8388, IF=2.161]

15. A. Shankar, **D. P. Rai**, Sandeep and R. K. Thapa, "Structure, electronic, magnetic and optical properties of neodymium chalcogenides" *Journal of Semiconductor* 33 (2012) 082001-6. [ISSN: 1674-4926]

16. **D. P. Rai** and R. K. Thapa, "A half-metallic ferromagnetism study of Co_2YAl (Y = Zr, Nb, Hf)based on GGA" *J. Spintron. Magn. Nanomater* 1 (2012) 97-103. [ISSN: 2158-866X]

17. **D. P. Rai** and R. K. Thapa, "A ground state study of X_2YZ (X = Co, Y=Mn, Z = Ge, Sb) by using LSDA+U method" *J. Adv. Phys.* 1(2) (2012) 126-131. [ISSN: 2168-1996]
18. **D. P. Rai**, A. Shankar, Sandeep, T. Malsawmtluanga, B. Vanlalruata, S. Gurung, L. R. Singh, M. Jamal, M. P. Ghimire and R. K. Thapa, "Calculation of Coulomb Repulsion (U) for 3d transition elements in Co_2YAl type Heusler alloys" *Armenian Journal of Physics* 5(3), (2012) 105-110. [ISSN 1829-1171]
19. **D. P. Rai** and R. K. Thapa, "A first principle calculation of full-Heusler alloy Co_2TiAl: LSDA+U Method." *ISRN Jour. Cond. Matter* 2012 (2012) 410326. [ISSN: 2090-7397]
20. **D. P. Rai** and R. K. Thapa, "Prediction of semiconducting behavior in minority spin of Co_2CrZ (Z = Ga, Ge, As):LSDA" *Journal of Semiconductor* 33 (2012) 1-6. [ISSN: 1674-4926]
21. **D. P. Rai**, A. Shankar, Sandeep, M. P. Ghimire and R. K. Thapa, "Study of Heusler compounds Co_2YSi (Y = Mn, Cr) using a full potential linearized augmented plane wave (FP-LAPW) method", M. *J. Condensed Matter* 14 (2012) 1-6. [ISSN: 1114-2073]
22. **D. P. Rai** and R. K. Thapa, "A first principle study of Co_2MnGe a Heusler compound" *Material Science: An Indian Journal* 9(2), (2012) 67-72. [ISSN 0974 7486]

2013

23. **D. P. Rai** and R. K. Thapa, "A density functional theory study of half-metallic ferromagnets (HMFs) behaviour in Co_2YSb" *Chinese Journal of Physics* 51(4) 795-804 (2013). [ISSN. 0577-9073, IF=0.48]
24. **D. P. Rai** and R. K. Thapa, "An ab initio study of half-metallic properties of Co_2TGe (T= Sc, Ti, V, Cr, Mn, Fe):LSDA+U method" *J. Korean Physical Society* 62 (11) (2013) 1652-1660.[ISSN: 1976-8524, IF=0.506]
25. **D. P. Rai** and R.K. Thapa, "A First Principle Study of Co_2CrZ (Z = In, Sn, Sb) Based on FP-LAPW Method" *Journal of Superconductivity and Novel Magnetism* 26 (6) (2013).[ISSN: 1557-1947, IF=0.702]
26. A. shankar, **D. P. Rai**, Sandeep and R. K. Thapa, "Ground state properties of filled skutterudite $EuFe_4P_{12}$: A first principles study" *Journal of Alloys and Compounds* 578925 559-564 (2013).[ISSN: 0925-8388, IF=2.161]

2014

27. **D. P. Rai**, J. Maibam, B. I. Sharma, A. Shankar, RK Thapa, S. H. Ke "Prediction of Half-metallic ferromagnetism (HMF) in hypothetical Heusler compound Co_2VSb using modified Becke Johnson (mBJ) potential" *Journal of Alloys and Compounds* 589,553-557 (2014). [ISSN: 0925-8388, IF=2.161]
28. **D. P. Rai** and R. K. Thapa Study of electronic, magnetic, optical and elastic properties of Cu_2MnAl a gapless full Heusler compound *Journal of Alloys and Compounds* 612, 355 (2014). [ISSN: 0925-8388, IF=2.161]
29. **D. P. Rai**, M. P. Ghimire and R. K. Thapa A DFT study of BeX (X = S, Se, Te) semiconductor: modified Becke Johnson (mBJ) potential *Semiconductors* 48, 1447 (2014) [IF=0.66]
30. **D. P. Rai** and R. K. Thapa, A Theoretical Study of Bulk Tungsten (W) Based on Momentum Transfer (q-Dependent) *Advances in Optics* 2014 9 (2014).
31. **D. P. Rai**, A. Shankar, Sandeep, L. R. Singh, B. I. Sharma, M. P. Ghimire and R. K. Thapa "Study of half-metallic properties of Co_2YGe (Y=Sc, Ti, V, Cr, Mn, Fe): A density functional theory (DFT)" *Journal of Physical Sciences* 25 45-57, (2014) [ISSN: 1675-3402]

2015

32. A. Shankar, **D. P. Rai**, R. Khenata, J. Maibam and R. K. Thapa Study of 5f electron based filled skutterudite compound $EuFe_4Sb_{12}$, a thermoelectric (TE) material: FP-LAPW method *Journal of Alloys and Compounds* 619, 621-626 (2015) [ISSN: 0925-8388, IF=2.161]
33. M. P. Ghimire, R. K. Thapa, **D. P. Rai**, T. P. Sinha, and Xiao Hu "Half metallic ferromagnetism in tri-layered perovskites $Sr_4T_3O_{10}$(T = Co, Rh)" *Journal of Applied Physics* 117, 063903 (2015)[IF:2.26]

34. A. Shankar, **D. P. Rai**, Sandeep and R. K. Thapa, "Investigation of elastic and optical properties of $EuFe_4P_{12}$ by first principles calculation" *Ind. J. Phys.* DOI:10.1007/s12648-015-0652-5, (2015)

35. **D. P. Rai**, A. Shankar, Sandeep, M. P. Ghimire and R. K. Thapa The electronic, magnetic and optical properties of double perovskite A_2FeReO_6 (A = Sr, Ba) from first principles approach *Comput. Mater. Sci.* 101, 313320 (2015)[Impact factor:1.897]

36. Sandeep, A. Shankar, **D. P. Rai**, M. P. Ghimire, R. Khenata and R. K. Thapa "Study of electronic and magnetic properties in $4f$ electron based cubic $EuAlO_3$: a first principles calculation" *Physica Scripta* 90, 065803 (2015)[ISSN: 1402-4896, IF=1.26].

37. A. Shankar, **D. P. Rai**, Sandeep, J. Maibam, R. Khenata, and R. K. Thapa "Elastic and Optical Properties of Filled Skutterudite $EuRu_4P_{12}$" *Chinese Journal of Physics* 53, 040804-9 (2015)[ISSN. 0577-9073,IF=0.48].

38. **D. P. Rai**, A. Shankar, Sandeep, M. P. Ghimire, R. Khenata and R. K. Thapa "Study of electronic and an enhanced thermoelectric properties of $Zr_xHf_{1-x-y}Ta_yNiSn$: A first principles study" *RSC Advances* 5, 95353-95359 (2015) DOI:10.1039/C5RA12897H [IF=3.87].

39. R. Moussa, A. Abdiche, R. Khenata, **D. P. Rai**, W. K. Ahmed, S Bin Omran, G. Murtaza and F. Soyalp "Studying structural, electronic and optical properties of zinc-blende $Ga_{1x}Al_xP$ at normal and under pressure by means of first principle" *Materials Research Express (IOP)* 2,105904 (2015).

2016

40. **D. P. Rai**, Sandeep, A. Shankar, M. P. Ghimire, R. Khenata and R. K. Thapa "Ferromagnetism in d^0 Binary Compounds MC (M = Be, Mg, Ca, Sr, Ba and Ra): A Modified Becke Johnson Potential Study" J*ornal of Advanced Physics* 5, 1-7, (2016).

41. A. Shankar, **D. P. Rai**, Sandeep, M. P. Ghimire, H. Joshi, R. Khenata and R. K. Thapa "Energy band structure, elastic and optical constants of the filled skutterudite $CeRu_4As_{12}$" -tMaterials Science in Semiconductor Processing 46, 10-16 (2016).

42. A. Shankar, **D. P. Rai**, Sandeep, M. P. Ghimire, H. Joshi, R. Khenata, R. K. Thapa and P. K. Mandal "Electronic structure and thermoelectricity of filled skutterudite $CeRu_4As_{12}$" *Journal of Alloys and Compounds* doi:10.1016/j.jallcom.2016.02.192.

43. F. Dahmane, Y. Mogulkoc, B. Doumi, A. Tadjer, R. Khenata, S. Bin Omran, **D.P. Rai**, G. Murtaza and Dinesh Varshney "Structural, electronic and magnetic properties of Fe_2-based full Heusler alloys: A first principle study" *Journal of Magnetism and Magnetic Materials* 407, 167-174 (2016).

Conference Proceedings

1. **D. P. Rai**, Sandeep, M.P. Ghimire and R.K. Thapa, "Electronic structure and magnetic properties of Co_2TiAl: A LSDA+U Study", *Crystal Growth and Computational Material Science Proceeding McMillan series* ISBN-978-935-059-048-5 (2011) 257-262.

2. **D. P. Rai**, Sandeep, M. P. Ghimire and R. K. Thapa "Ground state study of Electronic and Magnetic Properties of Co_2MnZ (Z = Ge, Sn) type Heusler Compounds : A first Principle Study" *Journal of Physics: Conference Series* 377 (2012) 012074-4.

3. Sandeep, M. P.Ghimire, **D. P. Rai**, P. K. Patra, A. K. Mohanty and R. K. Thapa, "Study of Bulk modulus, Volume, Energy, lattice parameters and magnetic moments in rare earth hexaborides using density functional theory" *Journal of Physics: Conference Series*377 (2012) 012084-3.

4. Sandeep, M. P. Ghimire, **D. P. Rai**, A. Shankar, A. K. Mohanty, Arthur Ernst, D. Deka, A. Rahman and R. K.Thapa "Electronic And Magnetic Properties Of $NdVSb_3$: A First Principles Study" *AIP Conf. Proc.* 1447 (2012) 1153-1154.

5. A. Shankar, **D. P. Rai**, Sandeep and R. K. Thapa Study of electronic and Magnetic properties of filled Skutterudite $EuFe_4P_{12}$: a first principle study *AIP Conf. Proc.* 1536, 437, 2013.

6. A. Shankar, **D. P. Rai**, Sandeep and R. K. Thapa Study of electronic and Magnetic properties of Ni_2MnGa by using LSDA+U method *Journal of Science Forum* 3 (1) 25-29, 2012.

7. D. Deka, A. Shankar, **D. P. Rai**, Sandeep, A. Rahman and R. K. Thapa Study of density of states and energy band structure in Bismuth Selenide *Journal of Science Forum* 3 (1) 19-20, 2012.

8. A. Shankar, **D. P. Rai**, Sandeep and R. K. Thapa, "A first principles calculation of ferromagnetic $EuFe_4Sb_{12}$" *Physics Procedia* 54, 127-131, 2014.

9. Sandeep, **D. P. Rai**, A. shankar, M. P. Ghimre and R. K. Thapa "Study of the electronic

and magnetic properties of $EuAlO_3$ using FP-LAPW method" *AIP Conference Proceedings* 1661, 070012, 2015.
10. R. Lalngaihawmi, B. Vanlalruata, A. Shankar, **D. P. Rai**, Sandeep, and R. K. Thapa "Study of aluminium pnictides by using full potential linearized augmented plane wave (FP-LAPW) method" *AIP Conference Proceedings* 1661, 050006, (2015).
11. A. Shankar, **D. P. Rai**, Sandeep, J. Maibam and R. K. Thapa "A first principles investigation of ferromagnetic $EuFe_4As_{12}$" *AIP Conference Proceedings* 1661, 070010, 2015.

List of Conferences attended

National Conferences

1. National Conference on Condensed Matter Days (CMDAYS), A first principle study of Rare Earth hexaborides (RB_6), **D. P. Rai**, Sandeep, M.P. Ghimire and R.K. Thapa, Kalyani University, Kolkata, 25-27th August (2010).
2. National Conference on Current Trend in Condensed Matter Physics (NCTCMP), Study of the Half metal based Heusler alloys: The case of NiVSb and NiTbSb. **D. P. Rai**, Sandeep, M.P. Ghimire and R.K. Thapa, Assam University, Silchar, 3-5th February (2011).
3. National Conference, Colloquium for Young Physicists (CYP), Electronic structure and magnetic properties of Co_2MnGe and Co2MnSb by using LSDA+U method, **D. P. Rai**, Sandeep, M.P. Ghimire and R.K. Thapa, SINP, Kolkata, 18-19th August (2011). 4. National Conference on Condensed Matter Days (CMDAYS), **D. P. Rai**, Sandeep, M.P. Ghimire and R.K. Thapa, Gauhati University, Guwahati, 24-26th August (2011).
5. National Conference on Solid State Symposium (DAE-SSPS), Electronic and magnetic properties of $NdVSb_3$: A First Principles Study, **D. P. Rai**, Sandeep, M.P. Ghimire and R.K. Thapa, SRM University, Kattankulathur, 19th-23rd December (2011).
6. National Conference on Condensed Matter Physics, A density functional study of Co_2YAl(Y=Zr, Nb)based on GGA. **D. P. Rai**, A. Shankar, Sandeep and R.K. Thapa, Birla Institute of Technology, Mesra, Ranchi 29-31 August 2012.
7. National Conference on Physics Academy of North East India, Study of Half metallic ferromagnetism (HMF) in Co_2CrBi a full-Heusler compound. **D. P. Rai**, A. Shankar, Sandeep, M. P. Ghimire and R. K. Thapa, Department of Physics, Mizoram University, Aizawl 17-19, December, 2012.
8. National Conference on Theoretical Physics, Study of Half Metal Ferromagnetism (HMF) in Transition Metal based Full-Heusler compound Co_2CrAl, **D. P. Rai**, A. Shankar, Sandeep, M. P. Ghimire and R. K. Thapa, Department of Physics, Tezpur University, Tezpur, 8-12 February, 2012.
9. *Science Academies Refresher Course in Experimental Physics* 8-23 March, 2016, Department of Physics, Tripura University, Agartala, India.

International Conferences

1. International Conference on Current Trend in Condensed Matter Physics (ICTCMP), DOS and band structure study of X_2YZ (X=Co, Y=Mn, Cr, Z=Si) Heusler alloys: A first principles method, **D. P. Rai**, Sandeep, M.P. Ghimire and R.K. Thapa, NISER, Bhubaneswar, 15-19th December (2010).
2. International Conference on Advance Materials (ICAM), Electronic structure and magnetic properties of Co_2TiAl: A LSDA+U Study, **D. P. Rai**, Sandeep, M.P. Ghimire and R.K. Thapa, PSG Tech College, Coimbatore, 12-16th December (2011).
3. International Conference (AIRAPT), Electronic Structure and Magnetic Properties of X_2YZ (X=Co, Y=Cr, Z=Al, Ga) type Heusler Compounds: A first Principle Study, **D. P. Rai**, Sandeep, M.P. Ghimire and R.K. Thapa, BARC, Mumbai, (2011).
4. International Conference on Recent Trends in Applied Physics and Material Science, An investigation of semiconducting behavior in minority spin of Co_2ScSb a full-Heusler compound. **D. P. Rai**, A. Shankar, Sandeep, M. P. Ghimire and R. K. Thapa, Govt. College of Engineering and Technology, Bikaner 01-02 February 2013.
5. International Conference on Nanoscience, Nanotechnology & Advanced Materials, A First Principles Study of Structural, Electronic and Optical properties of Aluminium Antimonide with Spin Orbit Coupling (SOC). **D. P. Rai**, A. Shankar, Sandeep, M. P. Ghimire and R. K. Thapa, Department of Chemistry, GITAM Institute of Science, Visakhapatnam 14-17 December 2015.

Workshop attended

1. State Level Workshop on FORTRAN Programing, Mizoram University, Aizawl, 24-26th November 2010.
2. National Workshop on Computational Physics, Mizoram University, Aizawl, 14-19th February 2011.
3. Advances in Electronics, Communication and Information Technology (AECIT), Mizoram University, Aizawl, 23rd-26th March (2011).
4. State Level Seminar on Recent Advances in Radiation Physics. Mizoram University, Aizawl, April 2011.
5. Workshop on Modelling biological Systems II, Department of Physics Mizoram University, Aizawl, 21-25 August 2012.
6. Workshop on statistical Programming-SSPS, North East Centre For Research and Development (NECRD) Indra Gandhi National Open University (IGNOU), Guwahati. 12-14 February 2013.
7. Workshop on Mathematical analysis, Department of Mathematics, Mizoram University, Aizawl, 7-8 March 2013.
8. Workshop on C^{++} Language and Numerical Methods, Department of Physics Pachhunga University college, 16-20, Feb, 2015.

National/International Collaborations

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