**Curriculum Vitae**

****

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- 1991-1995, High school Diploma, Amir Kabir High School Of Ghochan, Iran

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- 2001-2003,M.Sc. Physics, First class Honor , Ferdowsi University of Mashhad, Iran

- 2004-2009,Ph.D. Physics, First class Honor, Ferdowsi University of Mashhad, Iran

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- Distinguished **B.Sc.** Degree, Ferdowsi University of Mashhad, Iran (2000).

- Distinguished **M.Sc.** Degree, Ferdowsi University of Mashhad, Iran (2003).

- Distinguished **Ph.D.** Degree, Ferdowsi University of Mashhad, Iran (2009).

- Best Researcher in Hakim Sabzevari University of Sabzevar, Iran (2012).

- The top 2% of scientists in the world (2020).

**Publications:**

1. Ghorbani-Moghadam, T., HA Rahnamaye Aliabad, and M. Mousavi. "Optoelectronic properties of La2CoO4 and LaSrCoO4 Ruddlesden-Popper compounds: Comparative experimental and DFT studies by GGA/MBJ+ U." *Materials Science and Engineering: B* 286 (2022): 116074.
2. Azadparvar, Maliheh, M. Kheirabadi, and H. A. Aliabad. "Fluorinated derivatives of tetrahydroaltersolanol molecule on COVID-19, HIV, and HTLV protease by DFT and molecular docking approaches." *Journal of Molecular Modeling* 28, no. 11 (2022): 1-18.
3. Amiri-Shookoh, F., H. A. Aliabad, and H. Tavakoli-Anbaran. "Comparative DFT calculations on Bismuth-based compounds: new connection between optoelectronic properties and 209Bi and 51 V NMR and EFG." *Indian Journal of Physics* (2022): 1-11.
4. Aliabad, HA Rahnamaye, H. Vahidi, M. Samsami, Iftikhar Ahmad, and Gulten Kavak Balci. "Thermoelectric, optoelectronic and magnetic properties of BaLn2ZnO5 (Ln= Eu, Pr, Sm) insulators by GGA/mBJ+ U exchange-correlation approaches." *Materials Science and Engineering: B* 283 (2022): 115772.
5. Azadparvar, Maliheh, HA Rahnamaye Aliabad, E. Rezaei-Seresht, and M. Mirzaei. "Effect of fluorine substitution on the photobiological and electronic properties of resveratrol crystal structure: A first-principles study." *Journal of Photochemistry and Photobiology A: Chemistry* 429 (2022): 113941.
6. Rahnamaye Aliabad, H. A., H. Vahidi, Muhammad Khalid, M. Samsami, and Rifat Jawaria. "The electronic structure of graphene like C20H10CdN6O8. 5 metal–organic nanotube (MONT) based on FP-LAPW: for optoelectronic and thermoelectric devices." *Optical and Quantum Electronics* 54, no. 7 (2022): 1-10.
7. Aliabad, HA Rahnamaye, and H. Vahidi. "Optoelectronic properties of C 66 H 54 Br 6 N 6 O 12 supramolecular nanotube by DFT studies." (2022).
8. Amiri-Shookoh, F., H. A. Rahnamaye Aliabad, H. Tavakoli-Anbaran, and M. Samsami. "Optical, electronic structure, magnetic, NMR and hyperfine field properties of BiMPO5 and BiM2PO6 compounds (M= Ni, Co, Mn, Cu): a comparative DFT study." *Optical and Quantum Electronics* 54, no. 6 (2022): 1-19.
9. Samsami, M., Behnam Azadegan, H. A. Rahnamaye Aliabad, and F. Amiri-Shookoh. "DFT investigations of AgMC7H10N2 (M= Cl, Br, and I) metal organic molecules: NMR, optoelectronic, and transport properties." *Journal of Molecular Modeling* 28, no. 6 (2022): 1-15.
10. Bashi, M., Hossein Asghar Rahnamaye Aliabad, and M. Samsami. "Comparative studies of C7H10N2 pyridine and C7H10N2S pyrrole for optoelectronic applications by mBJ approach." *Journal of Molecular Modeling* 27, no. 9 (2021): 1-10.
11. Rahnamaye Aliabad, Hossein Asghar, and Mohammad Chahkandi. "IInvestigation of Non-Covalent Interactions and Optical Properties in a Manganese (II) Complex with Pyridine-N-oxide-2-carboxylic Acid." *Nashrieh Shimi va Mohandesi Shimi Iran* 40, no. 2 (2021): 195-207.
12. Bashi, Maryam, and Hossein Asghar Rahnamaye Aliabad. "Optoelectronic and thermoelectric properties of DMAP flexible compound for electronic devices by DFT." *Optical and Quantum Electronics* 53, no. 4 (2021): 1-12.
13. Maleki, Behrooz, Esmail Rezaei Seresht, Asma Baghdar Farooji, Hossein Asghar Rahnamaye Aliabad, Ali Jamshidi, and Hamid Reza Saadati Moshtaghin. "Effective Method for Knoevenagel Condensation Catalyzed by Acetoguanamine Supported on Magnetic Nanoparticles." *Nashrieh Shimi va Mohandesi Shimi Iran* 39, no. 4 (2021): 49-59.
14. Aliabad, HA Rahnamaye, M. Mousavi, and A. Abareshi. "First-principles calculations of optoelectronic and thermoelectric properties of HgGa2S4 chalcopyrite under pressure effect." *Materials Science and Engineering: B* 272 (2021): 115336.
15. Shookoh, F. Amiri, Hossien Tavakoli-Anbaran, and HA Rahnamaye Aliabad. "31P nuclear magnetic resonance, optical and thermal spectra in MP3 (M= Ir, Co, Rh, Ni) compounds by DFT." *Computational and Theoretical Chemistry* 1186 (2020): 112902.
16. Khalid, Muhammad, Akbar Ali, Jahrukh Tariq, Muhammad Nawaz Tahir, Hossein Asghar Rahnamaye Aliabad, Ishtiaq Hussain, Muhammad Ashfaq, and Muhammad Usman Khan. "Stabilization of Supramolecular Assembly of N‐Substituted Benzylidene Acetohydrazide Analogs by Non‐Covalent Interactions: A Concise Experimental and Theoretical Approach." *ChemistrySelect* 5, no. 34 (2020): 10618-10631.
17. Akram, Muhammad, Muhammad Adeel, Muhammad Khalid, Muhammad Nawaz Tahir, Hossein Asghar Rahnamaye Aliabad, Malik Aman Ullah, Javed Iqbal, and Ataualpa AC Braga. "Highly efficient one pot palladium-catalyzed synthesis of 3, 5-bis (arylated) pyridines: Comparative experimental and DFT studies." *Journal of Molecular Structure* 1213 (2020): 128131.
18. Maleki, Behrooz, Ehsan Esmaeilnezhad, Hyoung Jin Choi, Ehsan Koushki, Hossein Asghar Rahnamaye Aliabad, and Mozafar Esmaeili. "Glutathione-capped core-shell structured magnetite nanoparticles: Fabrication and their nonlinear optical characteristics." *Current Applied Physics* 20, no. 6 (2020): 822-827.
19. Bashi, M., and H. A. Rahnamaye Aliabad. "Investigation of 205Tl NMR shielding, structural, and electronical properties in thallium halides by applying PBE‐GGA, YS‐PBE0 and mBJ functionals." *Magnetic Resonance in Chemistry* 58, no. 3 (2020): 223-231.
20. Khan, Burhan, Muhammad Khalid, Muhammad Raza Shah, Muhammad Nawaz Tahir, Hafiz Muhammad Asif, Hossein Asghar Rahnamaye Aliabad, and Ajaz Hussain. "Synthetic, spectroscopic, SC-XRD and nonlinear optical analysis of potent hydrazide derivatives: a comparative experimental and DFT/TD-DFT exploration." *Journal of Molecular Structure* 1200 (2020): 127140.
21. Rahnamaye Aliabad, Hossein Asghar, Zahra Nodehi, Behrooz Maleki, and Azam Abareshi. "Electronical and thermoelectric properties of half-Heusler ZrNiPb under pressure in bulk and nanosheet structures for energy conversion." *Rare Metals* 38, no. 11 (2019): 1015-1023.
22. Aliabad, H. A., and M. Bashi. "Cobalt phthalocyanine polymer for optoelectronic and thermoelectric applications." *Journal of Materials Science: Materials in Electronics* 30, no. 20 (2019): 18720-18728.
23. Aliabad, HA Rahnamaye, S. Rabbanifar, and Muhammad Khalid. "Structural, optoelectronic and thermoelectric properties of FeSb2 under pressure: bulk and monolayer." *Physica B: Condensed Matter* 570 (2019): 100-109.
24. Bashi, M., HA Rahnamaye Aliabad, and B. Maleki. "Comparison between optoelectronic spectra and NMR shielding in tellurium based compounds: a FP-LAPW study." *Materials Research Express* 6, no. 10 (2019): 106314.
25. Chahkandi, Mohammad, and Hossein Asghar Rahnamaye Aliabad. "Crystalline network form of Gefitinib molecule stabilized by non–covalent interactions: DFT–D calculations." *Chemical Physics* 525 (2019): 110418.
26. Aliabad, H. A., and M. Chahkandi. "Theoretical study of crystalline network and optoelectronic properties of erlotinib hydrochloride molecule: non-covalent interactions consideration." *Chemical Papers* 73, no. 3 (2019): 737-746.
27. Rahnamaye Aliabad, Hossein Asghar, Zahra Sabazadeh, and Azam Abareshi. "Electronic structure and thermal properties of bulk and nano-layer of TAlO2 (T= Cu, Ag and Au) delafossite oxides." *Rare Metals* 38, no. 10 (2019): 905-913.
28. Saeed, Muhammad, Banaras Khan, Iftikhar Ahmad, Awais Siddique Saleemi, Najeebur Rehman, HA Rahnamaye Aliabad, and Sarir Uddin. "Theoretical investigations of thermoelectric phenomena in binary semiconducting skutterudites." *RSC advances* 9, no. 43 (2019): 24981-24986.
29. Aliabad, HA Rahnamaye. "Theoretical and experimental studies of La-substituted In2O3 nano-layer via the modified Becke-Johnson (mBJ) potential." *Optik* 175 (2018): 268-274.
30. Maleki, Behrooz, Sedigheh Ayazi Jannat Abadi, Mehdi Baghayeri, Hossein Asghar Rahnamaye Aliabad, and Hojat Veisi. "One-pot and three-component of tetrahydrobenzo [b] pyran derivatives using heterogeneous and recyclable catalysts and its application toward silver nanoparticle synthesis." *Applied Chemistry* 13, no. 48 (2018): 209-230.
31. Aliabad, HA Rahnamaye, and F. Asadi Rad. "Structural, electronic and thermoelectric properties of bulk and monolayer of Sb2Se3 under high pressure: By GGA and mBJ approaches." *Physica B: Condensed Matter* 545 (2018): 275-284.
32. Jbara, Ahmed S., Zulkafli Othaman, H. A. Aliabad, and M. A. Saeed. "Investigation of Electronic and Optical Properties of γ-and-Alumina by First Principle Calculations." *Advanced Science Letters* 24, no. 5 (2018): 3579-3581.
33. Chahkandi, Mohammad, and H. A. Rahnamaye Aliabad. "Role of hydrogen bonding in establishment of a crystalline network of Cu (II) complex with hydrazone-derived ligand: optoelectronic studies." *Chemical Papers* 72, no. 5 (2018): 1287-1297.
34. Rahnamaye Aliabad, H. A., and N. Hosseini. "Effect of substituted Ca on the thermoelectric and optoelectronic properties of NaRh2O4 under pressure." *Journal of Electronic Materials* 47, no. 3 (2018): 2009-2016.
35. Iqbal, R., M. Bilal, S. Jalali-Asadabadi, H. A. Rahnamaye Aliabad, and Iftikhar Ahmad. "Theoretical investigation of thermoelectric and elastic properties of intermetallic compounds ScTM (TM= Cu, Ag, Au and Pd)." *International Journal of Modern Physics B* 32, no. 02 (2018): 1850004.
36. Amiri, M. M., F. Amiri, F. Foroutan, and H. Asghar Rahnamaye Aliabad. "Effect of substituted Mn on optical properties of indium oxide and zinc oxide." *Bulg. Chem. Commun* 50 (2018): 335-340.
37. Aliabad, HA Rahnamaye, and M. Chahkandi. "Optoelectronic and structural studies of a Ni (II) complex including bicyclic guanidine ligands: DFT calculations." *Computational and Theoretical Chemistry* 1122 (2017): 53-61.
38. Bashi, Maryam, HA Rahnamaye Aliabad, Ali Asghar Mowlavi, and Iftikhar Ahmad. "125Te NMR shielding and optoelectronic spectra in XTe3O8 (X= Ti, Zr, Sn and Hf) compounds: Ab initio calculations." *Journal of Molecular Structure* 1148 (2017): 223-230.
39. Rahnamaye Aliabad, H. A., S. Basirat, and Iftikhar Ahmad. "Structural, electronical and thermoelectric properties of CdGa2S4 compound under high pressures by mBJ approach." *Journal of Materials Science: Materials in Electronics* 28, no. 21 (2017): 16476-16483.
40. Rahnamaye Aliabad, H. A., and Battal G. Yalcin. "Optoelectronic and thermoelectric response of Ca5Al2Sb6 to shift of band gap from direct to indirect." *Journal of Materials Science: Materials in Electronics* 28, no. 20 (2017): 14954-14964.
41. Abareshi, A., and HA Rahnamaye Aliabad. "Anisotropic thermoelectric properties of Sr5Sn2As6 compound under pressure by PBE-GGA and mBJ approaches." *Materials Research Express* 4, no. 9 (2017): 096303.
42. Rahnamaye Aliabad, H. A., Hamide Vaezi, Shiva Basirat, and Iftikhar Ahmad. "Role of the crystal lattice constants and band structures in the optoelectronic spectra of CdGa2S4 by DFT approaches." *Zeitschrift für anorganische und allgemeine Chemie* 643, no. 13 (2017): 839-849.
43. Amiri, Fatemeh, Fatemeh Foroutan, Mir Masumeh Amiri, and Hossein Asghar Rahnamaye. "Effect of Substituted Mn on Electronic Characteristics of Indium Oxide and Zinc Oxide via Density Functional Theory Studying." *Indian Journal of Science and Technology* 10 (2017): 13.
44. Jbara, Ahmed S., Zulkafli Othaman, H. A. Aliabad, and M. A. Saeed. "Electronic and Optical Properties of γ-and-Alumina by First Principle Calculations." *Advanced Science, Engineering and Medicine* 9, no. 4 (2017): 287-293.
45. Banaras Khan, H.A. Rahnamaye Aliabad, Imad Khan, S. Jalali-Asadabadi, Iftikhar Ahmad, *Comparative study of thermoelectric properties of Co based filled antimonide skutterudites with and without SOC effect*, Computational Materials Science 131, 308-314 (2017). (IF= 2.086)
46. H.A. Rahnamaye Aliabad, M. Chahkandi, *Comprehensive SPHYB and B3LYP−DFT studies of two types of Ferrocene,* [Zeitschrift für anorganische und allgemeine Chemie](http://onlinelibrary.wiley.com/journal/10.1002/(ISSN)1521-3749)*,* Inpress (2017). (IF= 1.251)
47. M. Bashi, H.A. Rahnamaye Aliabad, A. A. Mowlavi, Iftikhar Ahmad, *127I NMR calculations in binary metal iodides by PBE-GGA, YS-PBE0 and mBJ exchange correlation potentials,* Solid State Nuclear Magnetic Resonance 82-83*,* 10-15 (2017). (IF= 2.250)
48. M. Chahkandi, H.A. Rahnamaye Aliabad, *Evaluation of Non-covalent Binding Energies and Optoelectronic Properties of New CuBr2(C6H7N)2Complex: DFT Approaches,* [Zeitschrift für anorganische und allgemeine Chemie](http://onlinelibrary.wiley.com/journal/10.1002/(ISSN)1521-3749) 643, 180-191(2017). (IF= 1.251)
49. Banaras Khan, M. Yazdani-Kachoei, H.A. Rahnamaye Aliabad, Imad Khan,S. Jalali-Asadabadi, Iftikhar Ahmad, *Effects of chemical potential on the thermoelectric performance of alkaline-earth based skutterudites (AFe4Sb12, A=Ca, Sr and Ba)*, Journal of Alloys and Compounds 694, 253-260 (2017). (IF= 3.014)
50. H.A. Rahnamaye Aliabad , Z. Barzanuni , S. Ramezani Sani, Iftikhar Ahmad, S. Jalali-Asadabadi, H. Vaezi, M. Dastras, *Thermoelectric and phononic properties of (Gd, Tb)MnO3 compounds: DFT calculations*, Journal of Alloys and Compounds 690, 942-952 (2017). (IF= 3.014)
51. S. Bagci, Battal G. Yalcin, H. A. Rahnamaye Aliabad, S. Dumana, B. Salmankurt, *Structural, electronic, optical, vibrational and transport properties of CuBX2 (X = S, Se, Te) chalcopyrites*, RSC Adv. 6 , 59527- 59540 (2016). (IF= 3.289)
52. Gul Rehman, M. Shafiq, Saifullah, Rashid Ahmad, S. Jalali-Asadabadi, M. Maqbool, Imad Khan, H. A. Rahnamaye Aliabad, Iftikhar Ahmad, *Electronic Band Structures of the Highly Desirable III–V Semiconductors: TB-mBJ DFT Studies*, Journal of ELECTRONIC MATERIALS 45, 3314-3323 (2016). (IF= 1.491)
53. Battal G. Yalcin, M. Aslan, M. H. Ozcan, H. A. Rahnamaye Aliabad, *The optical spectrum of ternary alloy BBi1−xAsx*, Mater. Res. Express 3, 065901-9 (2016). (IF= 0.968)
54. Sardar Ahmad, Hamide Vaizie, H. A. Rahnamaye Aliabad, Rashid Ahmad, Imad Khan, Zahid Ali, S. Jalali-Asadabadi, Iftikhar Ahmad, Amir Abdullah Khan, *First-principles studies of pure and fluorine substituted alanines*, International Journal of Modern Physics B 30, 1650079-14 (2016). (IF= 0.94)
55. Imad Khan, Sajid Khan, Javid Iqbal, H. A. Rahnamaye Aliabad, Zahid Ali, Iftikhar Ahmad, *The Influence of Oxygen Substitution on the Optoelectronic Properties of ZnTe*, Journal of Chemistry 2016, 1-8 (2016). (IF= 0.772)
56. Junaid Munir, Ahmad Radzi Mat Isa, Masood Yousaf, H.A. Rahnamaye Aliabad, Qurat-ul Ain, M.A. Saeed, *Electronic, magnetic and optical properties of reduced hybrid layered complex Ni(pyz)V4O10 (pyz=C4H4N2) by first-principles*, Journal of Magnetism and Magnetic Materials 416, 241–246 (2016). (IF= 1.97)
57. H. A. Rahnamaye Aliabad, Z. Mojarradi, Battal G. Yalcin, *DFT studies for optoelectronic properties of pure L-alanine and doped with Li*, [Journal of Materials Science: Materials in Electronics](http://link.springer.com/journal/10854) 27, 4887-4897 (2016). (IF= 1.569)
58. Saeid Jalali Asadabadi, E. Ghasemikhah, T. Ouanhrani, M. Bayat Bayatani, S. Javanbakht, H. A. Rahnamaye Aliabad, Iftikhar Ahmad, J. Nematollahi, M. Yazdani Kachoei, *Electronic Structure of Crystalline Buckyballs: fcc-C60,* Journal of ELECTRONIC MATERIALS 45, 339-348 (2016). (IF= 1.798)
59. Imad Khan, Iftikhar Ahmad, H. A. Rahnamaye Aliabad, M. Maqboold, *DFT-mBJ studies of the band structures of the II-VI semiconductors,* Materials Today: Proceedings 2, 5122 – 5127 ( 2015 ).
60. H.A. Rahnamaye Aliabad, R. Tayebee, M. Boroumand Khalili, *Ab initio studies of optoelectronic properties of fluorine-substituted ferrocene,* [Research on Chemical Intermediates](http://link.springer.com/journal/11164) 42, 3743-3761(2015). (IF= 1.833)
61. H.A. Rahnamaye Aliabad, Battal G. Yalcin, *Effects of IIIB transition metals on optoelectronic and magnetic properties of HoMnO3: A first principles study,* Chin. Phys. B 24, 117102 (2015). (IF= 1.436)
62. H.A. Rahnamaye Aliabad, *Investigation of optoelectronic properties of pure and Co substituted a-Al2O3 by Hubbard and modified Becke–Johnson exchange potentials,* Chin. Phys. B 24, 097102 (2015). (IF= 1.436)
63. H.A. Rahnamaye Aliabad, H. Akbari, M.A. Saeed; *Evaluation of magneto-optic properties of LaXPO(X = Mn, Fe, Ni) new superconductors by DFT,* Computational Materials Science 106, 5-14 (2015). (IF= 2.086)
64. Masood Yousaf, S.A. Dalhato, G. Murtaza, R. Khenata, M. Sajjad, A. Musa, H.A. Rahnamaye Aliabad, M.A. Saeed; *Optoelectronic properties of XIn2S4 (X= Cd, Mg) thiospinels through highly accurate allelectron FP-LAPW method coupled with modified approximations*, Journal of Alloys and Compounds 625, 182-187 (2015). (IF= 3.014)
65. Banaras Khan, H.A. Rahnamaye Aliabad , N. Razghandi , M. Maqboold, S. Jalali Asadabadi, Iftikhar Ahmada, *Structural and thermoelectric properties of pure and La, Y doped HoMnO3 for their use as alternative energy materials*, Computer Physics Communications, 187, 1-7 (2015). (IF= 3.635)
66. M. Bilala, Saifullah, M.Shafiq, B. Khan, H.A.Rahnamaye Aliabad, S. Jalali Asadabadid, Rashid Ahmade, Iftikhar Ahmada, *Antiperovskite compounds SbNSr3 and BiNSr3: Potential candidates for thermoelectric renewable energy generators*, Physics Letters A 379, 206-210 (2015). (IF= 1.677)
67. M. Shafiq, Suneela Arif , Iftikhar Ahmad , S. Jalali Asadabadi , M. Maqbool , H.A. Rahnamaye Aliabad, *Elastic and mechanical properties of lanthanide monoxides*, Journal of Alloys and Compounds 618, 292-298 (2015). (IF= 3.014)
68. M. Jamal, S. Jalali Asadabadi, Iftikhar Ahmad , H.A. Rahnamaye Aliabad, *Elastic constants of cubic crystals*, Computational Materials Science 95, 592-599 (2014). (IF= 2.086)
69. H.A. Rahnamaye Aliabad, Z. Parvizi, *Structural, electronical and thermal properties of XVO4 (X = Y, Gd) vanadate crystals*, Computational Materials Science 93, 125–132 (2014). (IF= 2.086)
70. M. Bilal , Banaras Khan, H. A. Rahnamaye Aliabad, M. Maqbool, S. Jalali Asadabadi, Iftikhar Ahmad, *Thermoelectric properties of SbNCa3 and BiNCa3 for thermoelectric devices and alternative energy applications*, Computer Physics Communications, 185, 1394–1398 (2014). (IF= 3.635)
71. M. Bilal , Iftikhar Ahmad , H. A. Rahnamaye Aliabad , S. Jalali Asadabadi *, Detailed DFT studies of the band profiles and optical properties of antiperovskites SbNCa3 and BiNCa3*, Computational Materials Science 85, 310-315 (2014). (IF= 2.086)
72. H.A. Rahnamaye Aliabad, M. Kheirabadi, *Thermoelectricity and superconductivity in pure and doped Bi2Te3 with Se*, Physica B: Condensed Matter 433,157- 164 ( 2014). (IF= 1.352)
73. Zahid Ali, M. Shafiq, S. Jalali Asadabadi, H. A. Rahnamaye Aliabad, Imad Khan, Iftikhar Ahmad,*Magneto-electronic studies of anti-perovskites NiNMn3 and ZnNMn3*, Computational Materials Science 81, 141-145 (2014). (IF= 2.086)
74. Rashid Iqbal, Imad Khan, H. A. Rahnamaye Aliabad, Zahid Ali, Iftikhar Ahmad, *Density functional studies of magneto-optic properties of CdCoS*, Journal of Magnetism and Magnetic Materials 351, 60-64 (2014). (IF= 1.97)
75. H. A. Rahnamaye Aliabad, M. Bazrafshan, H. Vaezi, Masood Yousaf, Junaid Munir, M. A. Saeed, *"* Optoelectronic Properties of Pure and Co Doped Indium Oxide by Hubbard and modified Becke-Johnson Exchange Potentials", CHIN. PHYS. LETT. Vol. 30, No. 12, 127101-5 (2013). (IF= 0.875)
76. Imad Khan, H.A. Rahnamaye Aliabad, Waqar Ahmad, Zahid Ali, Iftikhar Ahmad, *First principle optoelectronic studies of visible light sensitive CZT*, Superlattices and Microstructures 63, 91–99 (2013). (IF= 2.117)
77. Masood Yousaf, M. A. Saeed, Ahmad Radzi Mat Isa, H. A. Rahnamaye Aliabad, M. R. Sahar "*An Insight into the Structural, Electronic and Transport Characteristics of XIn2S4 (X=Zn, Hg) Thiospinels using a Highly Accurate All-Electron FP-LAPW+Lo Method*", CHIN. PHYS. LETT. Vol. 30, No. 7, 077402 (2013). (IF= 0.875)
78. Imad Khan, Iftikhar Ahmad, H.A. Rahnamaye Aliabad, S. Jalali Asadabadi, Zahid Ali, M. Maqbool, *" Conversion of optically isotropic to anisotropic CdSxSe1-x (0 < x< 1) alloy with S concentration* ", Computational Materials Science 77, 145-152(2013). (IF= 2.086)
79. Zahid Ali, Imad Khan, Iftikhar Ahmad, S. Naeem, H. A. Rahnamaye Aliabad, S. Jalali Asadabadi, D. Zhang, *"* [*Comparison of the electronic band profiles and magneto-optic properties of cubic and orthorhombic SrTbO3*](http://www.sciencedirect.com/science/article/pii/S0921452613002603) ", Physica B: Condensed Matter 423,16-20 ( 2013). (IF= 1.352)
80. Zahid Ali, Sajad Ali, Iftikhar Ahmad, Imad Khan, H. A. Rahnamaye Aliabad, *"* [*Structural and optoelectronic properties of the zinc titanate perovskite and spinel by modified Becke–Johnson potential*](http://www.sciencedirect.com/science/article/pii/S0921452613002068) ", Physica B: Condensed Matter 420, 54-57 (2013). (IF= 1.352)
81. H. A. Rahnamaye Aliabad, V. Hesam, Iftikhar Ahmad, Imad Khan, "*Electronic band structure of LaCoO3/Y/Mn compounds* ", Physica B: Condensed Matter 410, 112-119 (2013). (IF= 1.352)
82. Imad Khan, Iftikhar Ahmad, D. Zhang, H. A. Rahnamaye Aliabad, S. Jalali Asadabadi ," *Electronic and optical properties of mixed Be-chalcogenides*", Journal of Physics and Chemistry of Solids 74,181-188 (2013). (IF= 2.048)
83. H. A. Rahnamaye Aliabad, M. Fathabadi, Iftikhar Ahmad, "*Optoelectronic Properties of KDP by First Principle Calculations* ", International Journal of Quantum Chemistry 113, 865-872 (2013). (IF= 2.184)
84. M. Yousaf, M. A. Saeed, A. R. MAT ISA, H. A. Rahnamaye Aliabad, N. A. NOOR, " *Ab initio study of optoelectronic properties of spinel ZnAl2O4 beyond GGA and LDA* ", International Journal of Modern Physics B, Vol. 26, No. 32 1250198 (2012). (IF= 0.94)
85. H. A. Rahnamaye Aliabad , M. Ghazanfari, Iftikhar Ahmad, M. A. Saeed, " *Ab initio calculations of structural, optical and thermoelectric properties for CoSb3 and ACo4Sb12 (A = La, Tl and Y) compounds* ", Computational Materials Science 65, 509-519(2012). (IF= 2.086)
86. Imad Khan, Iftikhar Ahmad, H. A. Rahnamaye Aliabad and M. Maqbool, "*Effect of phase transition on the optoelectronic properties of Zn1−xMgxS* ", JOURNAL OF APPLIED PHYSICS 112, 073104 (2012). (IF= 2.183)
87. Masood Yousaf, M. A. Saeed, Ahmad Radzi Mat Isa, Amiruddin Shaari, H. A. Rahnamaye Aliabad, "*Electronic Band Structure and Optical Parameters of Spinel SnMg2O4 by Modified Becke–Johnson Potential*", CHIN. PHYS. LETT. Vol. 29, No. 10, 107401(2012). (IF= 0.875)
88. Imad Khan, A. Afaq, H. A. Rahnamaye Aliabad, Iftikhar Ahmad, "*Transition from optically inactive to active Mg-chalcogenides: A first principle study* ", Computational Materials Science 61, 278-282 (2012). (IF= 2.086)
89. H. A. Rahnamaye Aliabad, Y. Asadi and Iftikhar Ahmad, "*Quasiparticle optoelectronic properties of pure and doped Indium Oxide*", Optical Materials 34, 1406–1414 (2012). (IF= 2.183)
90. H. A. Rahnamaye Aliabad, Iftikhar Ahmad," *Optoelectronic properties of LixAxNbO3 (A=Na, K, Rb, Cs, Fr) crystals*"*,* Physica B: Condensed Matter 407, 368- 377(2012). (IF= 1.352)
91. H. A. Rahnamaye Aliabad and H. Arabshahi, A. Hamel Aliabadi "The *effect of Hubbard potential on effective mass of carries in doped Indium Oxide*", International Journal of the Physical Sciences Vol. 7(5), 696-708 (2012). (IF= 0.37)
92. G. Murtaza, Iftikhar Ahmad, M. Maqbool, H. A. Rahnamaye Aliabad, A. Afaq, "*Structural and Optoelectronic Properties of Cubic CsPbF3 for Novel Applications*", CHIN. PHYS. LETT. Vol. 28, No. 11, 117803 (2011). (IF= 0.875)
93. G. Murtaza , G. Sadique , H. A. Rahnamaye Aliabad , M.N. Khalid , S. Naeem , A. Afaq , B. Amin , Iftikhar Ahmad, "*First principle study of cubic perovskites: AgTF3 (T=Mg, Zn)*", Physica B: Condensed Matter 406, 4584(2011). (IF= 1.352)
94. S. Arif, Iftikhar Ahmad, B. Amin, H. A. Rahnamaye Aliabad,"*Robust Half-Metallicity in a Chromium-Substituted AlN*", CHIN. PHYS. LETT. Vol. 28, No. 10,108501 (2011). (IF= 0.875)
95. H. A. Rahnamaye Aliabad, N. Mahmoodi and H. Arabshahi, "*The effect of magnetic impurity on the electronical and optical properties of corundum*", International Journal of the Physical Sciences Vol. 6(15), 3747-3755 (2011). (IF= 0.37)
96. H. A. Rahnamaye Aliabad, S. R. Ghorbani, "*Structural and Spin Polarization Effects of Cr, Fe and Ti Elements on Electronical Properties of α–Al2O3 by First Principle Calculations*", Journal of Modern Physics 2, 158-161 (2011). (IF= 0.43)
97. M. Ghasemifard, M. Zavar, H. Ghasemifard and H. A. Rahnamaye Aliabad, "*The effect of temperature dependences on optical properties of PMN-PZT nano-powders*", Journal of Optics 39, 157-166 (2010).
98. S. M. Hosseini, H. A. Rahnamaye Aliabad and A. Kompany," *Electronic and thermoelectric properties of pure and alloys In2O3 transparent conductors* ", Modern Physics Letters B, Vol. 24, No. 21, 2251–2265 (2010). (IF= 0.687)
99. H. A. Rahnamaye Aliabad, M. R. Benam and H. Arabshahi,*” Theoretical studies of the effect of Ti, Zr and Hf substitutions on the electronic properties of alpha alumina”*, International Journal of Physical Sciences Vol. 4 (8), 437-442, (2009). (IF= 0.37)
100. H. A. Rahnamaye Aliabad, S. M. Hosseini , A. Kompany, A. Youssefi , E. Attaran*,” Optical properties of pure and transition metal-doped indium oxide”,* Phys. stat. sol. (b), 246, No. 5, 1072-1081 (2009). (IF= 1.489)
101. H. Arabshahi, J. Baedi, H.A. Rahnamaye Aliabad, G.R. Ebrahimi, *“Potential performance of SiC and GaN based metal semiconductor field effect transisors”* Rom. Journ. Phys.,Vol. 54, 377–384 (2009). (IF= 1.398)
102. A. Kompany, H. A. Rahnamaye Aliabad, S. M. Hosseini, J. baedi, "*Effect of substituted IIIB transition metals on electronic properties of Indium Oxide by first principles calculations*". Phys.stat.sol. (b), 244, No. 2, 619–628 (2007). (IF= 1.489)
103. M. R. Benam, H.A.Rahnamaye Aliabad and S.M.Hosseini," *Effect of substituted IIIB transition metals on the energy gap of α–Al2O3 by first- principle calculations*", Phys. stat. sol. (a) 203, No.9, 2223-2228(2006). (IF= 1.648)
104. S.M.Hosseini, H.A.Rahnamaye Aliabad and A.Kompany," *First principle study of optical properties of pure α–Al2O3 and La aluminates*", Eur. phys.J.B 43, 439- 444 (2005). (IF= 1.345)
105. S.M.Hosseini, H.A.Rahnamaye Aliabad and A.Kompany," *Influence of La on electronic structure of α–Al2O3 High k-gate from first principle*", Ceramics International 31, 671-675 (2005). (IF= 2.758)

**Participate in Conferences:**

1. Z. Mouseli, **H. A. Rahnamaye Aliabad**,S. Jalali Asadabadi, "*Investigation of optoelectronic properties of XRuO3 (X=Ca, Sr) Compounds*", Proceeding of The 11th Condensed Matter Conference of the Physics Society of Iran, Shahrood University of Technology, Shahrood, Iran (26-27January) 2013
2. M. Rezvanian, S. Reesy, S. Jalali Asadabadi**, H. A. Rahnamaye Aliabad**,, "*Contributions of electrostatic and quantum interactions in the cooperativity of hydrogen bonds in polyalanine alphahelix*", Proceeding of The 11th Condensed Matter Conference of the Physics Society of Iran, Shahrood University of Technology, Shahrood, Iran (26-27January) 2013
3. Z. Barzanooni , **H. A. Rahnamaye Aliabad**, "*First principles study of electronic and optical properties of (R=Gd,Dy)RMnO3 compounds*", Proceeding of The 11th Condensed Matter Conference of the Physics Society of Iran, Shahrood University of Technology, Shahrood, Iran (26-27January) 2013
4. Z. Barzanooni , **H. A. Rahnamaye Aliabad**, "*Study of electronic and thermoelectric properties of TbMnO3* ", Proceeding of The 11th Condensed Matter Conference of the Physics Society of Iran, Shahrood University of Technology, Shahrood, Iran (26-27January) 2013
5. Z. Barzanooni , **H. A. Rahnamaye Aliabad**, "*In search of new thermoelectric materials based on GdMnO3 magnetite* ", Proceeding of The 11th Condensed Matter Conference of the Physics Society of Iran, Shahrood University of Technology, Shahrood, Iran (26-27January) 2013
6. **H. A. Rahnamaye Aliabad**; N. Razghandi; A. Askari; Iftikhar Ahmad; S. Jalali Asadabadi, "*The effect of Hubard potential on HoMnO3 optical spectrums*", Proceeding of Physics conference of Iran, Yazd (27-30 August 2012) 1376
7. **H. A. Rahnamaye Aliabad**; M. Fathabadi; A. Askari; Iftikhar Ahmad; S. Jalali Asadabadi, "*Optical properties of KDP by GGA and MBJGGA*", Proceeding of Physics conference of Iran, Yazd (27-30 August 2012) 1380
8. Rezvanian, Mahmood; Jalali Asadabadi, Saeid, Iftikhar Ahmad**, H. A. Rahnamaye Aliabad**; "*Cooperativity calculations of hydrogen bonds in polyalanine alphahelix*", Proceeding of Physics conference of Iran, Yazd (27-30 August 2012) 162
9. M. Yazdanmehr, S. Jalali Asadabadi, A. Nourmohammadi, Iftikhar Ahmad, **H. A. Rahnamaye Aliabad**;" *Electronic Structure and Band Gap Calculations of γ-Al2O3 Compound Using Modified Becke-Johnson (mBJ) Exchange Potent*", Proceeding of Physics conference of Iran, Yazd (27-30 August 2012) 1494
10. M. Yazdanmehr, S. Jalali Asadabadi, A. Nourmohammadi, Iftikhar Ahmad, **H. A. Rahnamaye Aliabad**;"*Effects Induced by Applying External Electric Field in GaAs Compound*", Proceeding of Physics conference of Iran, Yazd (27-30 August 2012) 1498
11. **H. A. Rahnamaye Aliabad**,"*Spin polarization in organometallic Ferrocene X(C5H5)2(X =Fe ,Mn ,Cr ,Co);* The effect of magnetic impurity on electronical properties of Indium Oxide in cubic and rombohedral phases*; Optoelectronic properties of YBCO and MgB2 superconductors; Spin polarization in pure LaCoO3 and doped with magnetic and nonmagnetic impurities;* The effect of magnetic impurity on electronical properties of Indium Oxide in cubic and rombohedral phases", The seventh international conference on magnetic and superconducting materials (MCSM11)25th August, Malaysia (2011)
12. **H. A. Rahnamaye Aliabad**, "Optical *properties of KDP in tetragonal crystal structure* ", proceeding of 6th International Conference on Photonics and Applications (ICPA6), Hanoi, Vietnam, (2010)
13. A. Kompany , S. M. Hosseini and **H .A. Rahnamaye Aliabad**, "*Study of the effect of IIIB transition metals on electronic properties of Indium oxide by first- principle calculations*". Proceeding of International conference on new energy materials, C145, Beijing, China, June 25-June 30, 2006
14. M. R. Benam and **H. A. Rahnamaye Aliabad**, "*Theoretical studies of the effect of Ti,Zr and Hf impurities on the electrical properties of Alpha-Alumina*", proceeding of DFTEM 2006-bringig together two communities, poster 117, April 21- 23, 2006,Vienna/Austria
15. **H. A. Rahnamaye Aliaba­d**, ,S M. Hosseini, " *First principle study of optical properties of pure α-Al2O3 and La aluminates*", Proceeding of 3rd international conference on material for advanced technology(ICMAT 2005), Oral presentation, Abstract id:conf 52 a 307, 3-8 July 2005, Singapore
16. S. M. Hosseini, **H. A. Rahnamaye Aliabad** and A. Kompany, "*First principle study of optical properties of pure α-Al2O3 and La aluminates*", Proceeding of International conference on smart materials (smart mat-04), Oral presentation, Cod No. 03-3-3, Ching mai, Thailand, (1-3 December 2004)
17. S. M. Hosseini, **H. A. Rahnamaye Aliabad** and A. Kompany," *Investigation of Optical properties and Electron Energy Loss of α-Al2O3*", Proceeding of 'the 11th symposium of the society crystallography and mineralogy of Iran, Yazd, (2004) 463

**Papers under review:**

Presently 5 papers are under review in different ISI journals.

**Research Students:**

35 MS students have completed their projects successfully. Now, 4 MS students are currently working with me at Hakim Sabzevari University, Iran. Also, 2 Ph. D students are currently working with me.

**Experiences:**

Experience Working with **WIEN2K, BOLTZTRAP** and **ABINIT** Codes (***calculation of electron density, density of state, electron energy loss near edge structure, optical properties, band structure, spin polarization, spin orbit interaction, Thermoelectric properties, …***)

**Field of interests:**

Density Functional Theory, Bulk and Surface physics, Nanotechnology, Semiconductors, Organometallic materials,druges, Ceramics and Superconductivity.