

Curriculum Vitae

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Education:

- 1991-1995, High school Diploma, Amir Kabir High School Of Ghochan, Iran
- 1996- 2000, B.Sc. Physics, First class Honor, Ferdowsi University of Mashhad, Iran
- 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

Awards and distinctions:

- 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 and 2022).
- The top 2% of scientists in the world (2020).

Publications:

1. Azadparvar, Maliheh, H. A. Rahnamaye Aliabad, and Evren G. Özdemir. "Optoelectronic and thermoelectric properties of Sb₂S₃ under hydrostatic pressure for energy conversion." *AIP Advances* 13, no. 6 (2023).
2. Rahnamaye Aliabad, H. A., Maliheh Azadparvar, Behnam Mahdavi, R. Golestani, Muhammad Khalid, and Z. Choopani. "First principle study of the optoelectronic properties of pyrazinamide drug." *Optical and Quantum Electronics* 55, no. 8 (2023): 714.
3. Azadparvar, Maliheh, HA Rahnamaye Aliabad, E. Rezaei-Seresht, Iftikhar Ahmad, and H. Sharafi. "Fluorine derivatives of piceatannol for photobiological and photophysical applications by DFT approach." *Chemical Physics Letters* (2023): 140732.
4. H. A. Rahnamaye Aliabad, B. Mahdavi, Maliheh Azadparvar, R. Golestani, Z. Choopani, DFT study of sertraline hydrochloride antidepressant drug, *Journal of Molecular Modeling* 29, no. 5 (2023): 144.
5. H. A. Rahnamaye Aliabad, Muhammad Aamir Iqbal, F. Amiri-Shookoh, Nadia Anwar, Sunila Bakhsh, and Iván D. Arellano-Ramírez, Effects of the Hubbard Potential on the NMR Shielding and Optoelectronic Properties of BiMnVO₅ Compound, *Scientific Reports* 13, no. 1 (2023): 5816.
6. 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* (2023): 797-807.
7. 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.
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9. Aliabad, HA Rahnamaye, H. Vahidi, M. Samsami, Iftikhar Ahmad, and Gulden 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.
10. 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.
11. 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.
12. Aliabad, HA Rahnamaye, and H. Vahidi. "Optoelectronic properties of C₆₆H₅₄Br₆N₆O₁₂ supramolecular nanotube by DFT studies." (2022).

13. 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.
14. 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.
15. 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.
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17. 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.
18. 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.
19. 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.
20. 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.
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23. 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.
24. 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.

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26. 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.
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55. 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)
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Participate in Conferences:

- 1) Z. Mouseli, **H. A. Rahnamaye Aliabad**, S. Jalali Asadabadi, "*Investigation of optoelectronic properties of $XRuO_3$ ($X=Ca, Sr$) 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 polyaniline 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 ($R=Gd,Dy$) $RMnO_3$ 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 $TbMnO_3$* ", Proceeding of The 11th Condensed Matter Conference of the Physics Society of Iran, Shahrood University of Technology, Shahrood, Iran (26-27January) 2013
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- 6) **H. A. Rahnamaye Aliabad**; N. Razghandi; A. Askari; Iftikhar Ahmad; S. Jalali Asadabadi, "*The effect of Hubard potential on $HoMnO_3$ 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 $X(C_5H_5)_2$ ($X = Fe, Mn, Cr, Co$); 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. Rahnemaye 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

Research Students:

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

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.