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		SCOPUS:	http://www.scopus.com/authid/detail.uri?authorId=56022641400

Status

Married having Two sons (Farhad and Mahdi)

Education

B.Sc.
Sharif University of Technology, Tehran, Iran 1985-1990
M.Sc.
Isfahan University of Technology, Isfahan, Iran 1996-1998
- **M.Sc. thesis:** Quantum Chaos in 3-Dimensional Stadium

Ph.D.
Isfahan University of Technology, Isfahan, Iran 1998-2003
- **Ph.D. thesis:** The valence of strongly correlated f-electron compounds from analysis of electric field gradients (EFG's)

Research

Computational condensed matter physics in the framework of the Density Functional Theory (DFT) using ab initio Full Potential (Linearized) augmented Plane Wave plus local orbital (FP-(L)APW+lo) method, employing WIEN2K code (http://www.wien2k.at) to calculate a broad range of solid sates properties of materials including strongly correlated and bio systems:

- ✓ Density Functional Theory (DFT)
- ✓ Crystal Field Theory (CFT)
- ✓ Combining Dynamical Mean Filed Theory (DMFT) with DFT
- ✓ Combining Boltzmann Theory (BT) with DFT
- ✓ Quantum Theory of Atoms in Molecules (QTAIM)
- ✓ Combining Eliashberg Theory with DFT for the Study of Superconductors

- ✓ Magnetism of isolated impurities in a transition metal host matrix
- ✓ Hyperfine Interactions: magnetic hyperfine fields (HFF) and electric field gradient (EFG)
- ✓ Nuclear Magnetic Resonance (NMR)
- ✓ Acoustic Properties (Elastic constants)
- ✓ Optical properties (Dielectric constants)
- ✓ Transport Properties (Electric, Magnetic, Thermal conductivities) using BoltzTrap code (Madsen, G. K. H.; Singh, D. J. *Comp. Phys. Commun.* **2006** 175, 67 http://arxiv.org/PS_cache/cond-mat/pdf/0602/0602203.pdf, http://www.chem.au.dk/~webuorg/new/groups/gm/BoltzTrap/BoltzTrap.html)
- ✓ Effects of lattice and/or atomic relaxation
- ✓ Effects of Hubbard U parameter
- ✓ Quantum size effects near the surfaces and/or interfaces of nanomaterials
- ✓ Spintronics (spin + electronics) in halfmetals
- ✓ Non-Collinear Magnetism using WIENncm code (http://www.wien2k.at/reg_user/ncm/)

Teaching

Courses

- ✓ Fundamental of Physics: R. A. Serway, J. W. Jewett and/or D. Halliday, R. Resnick, J. Walker
- ✓ Modern Physics: R. A. Serway, C. J. Moses, C. A. Moyer
- ✓ Solid state physics: C. Kittle (Undergraduate), N. W. Ashcroft and N. D. Mermin and/or G. Grosso, G. Parravicini, G. Pastori Parravicini (Graduate)
- ✓ Quantum Mechanics: S. Gasiorowicz (Undergraduate), L. E. Ballentine and/or J. J. Sakurai (Graduate)
- ✓ Statistical Mechanics: Berkeley Physics Course, Vol. 5 (Undergraduate) R. Pathria and/or L. E. Reichl (Graduate)
- ✓ Thermodynamics: M. W. Zemansky, Richard H. Dittman and/or L. E. Reichl
- ✓ Computational Physics: Numerical Recipes: http://www.nr.com
- ✓ Quantum Theory of Solid States
- ✓ Density functional theory, R. M. Martin and/or R. G. Parr, W. Yang
- ✓ Condensed matter physics

✓ Classical Mechanics: Keyth R. Symon

Referee of The Peer-Reviewed ISI Journals

- Journal of Physics: Condensed Matter
- Journal of Physics D: Applied Physics
- Journal of Physics B: Atomic, Molecular and Optical Physics
- ECS Journal of Solid State Science and Technology
- Nanotechnology
- Journal of Applied Physics
- Physical Chemistry Chemical Physics (PCCP)
- RSC Advances
- Philosophical Magazine Letters
- Journal of Magnetism and Magnetic Materials
- Thin Solid Films
- Journal of Alloys and Compound
- Crystal Research and Technology
- Journal of Materials Science: Materials in Electronics
- Rare Metals
- Journal of Physics and Chemistry of Solids
- Semiconductor Science and Technology
- Materials Research Express
- Materials Science in Semiconductor Processing
- Fuel Cells
- Computational Materials Science
- Computational Condensed Matter
- Physica Scripta
- Iranian Journal of Research Physics
- Journal of Research on Many-body Systems
- Indian Journal of Physics
- Pramana – Journal of Physics

Publication

1. S. Jalali Asadabadi, S. Cotteneer, H. Akbarzadeh, R. saki, and M. Rots, The Valency of Rare Earths in RIn3 and RSn3: ab initio Analysis of Electric-Field Gradients, Phys. Rev. B 66, 195103 (2002).
2. S. Jalali Asadabadi, H. Akbarzadeh, Density functional approach to study structural properties and electric field gradients in rare earth materials, Physica B 349, 76 (2004).
3. A. Fathi, S. Jalali Asadabadi, M. Goshtasbi Rad, Hyperfine Interactions in USb2 crystal, Iranian Journal of Physics, Vol. 2, No. 6, 123-136 (2006).

4. S. Jalali Asadabadi, Electronic structure and electric-field gradient analysis in CeIn3, Phys. Rev. B 75, 205130 (2007).
5. S. Jalali Asadabadi, Valence of cerium in CeIn3 metallic compound by electric-field gradients analysis from LDA+U calculations", research center, University of Isfahan, Isfahan, Iran, (2007).
6. M. Rafiee, S. Jalali Asadabadi, "First principle study of Pb/Si(111) interface", Iranian Journal of Physics Research Vol. 7, No. 3, 171-179 (2007).
7. M. Ilkhani, M. R. Abolhasani, S. Jalali Asadabadi, "Ab initio study of solid CeIn3 at high pressures", Iranian Journal of Physics Research Vol. 8, No. 2, 99-107 (2008).
8. A. R. Faghihi, S. Jalali Asadabadi, "Ab inito calculations of Hubbard parameters for NiO and Gd crystals", Iranian Journal of Physics Research Vol. 8, No. 3, 143-152 (2008).
9. F. Kheradmand, S. Jalali Asadabadi, "Structural and electronic properties of cerium from LDA+U calculations", Iranian Journal of Physics Research Vol. 8, No. 4, 235-240 (2008).
10. S Javanbakht, S Jalali Asadabadi, "Band structure of fcc-C60 solid state crystal study", Iranian Journal of Physics Research Vol. 9, No. 2, 301-308 (2009).
11. M. Rafiee, S. Jalali Asadabadi, "Quantum size effects in Pb/Si(111) thin films from density functional calculations", Computational Materials Science 47, 584 (2009).
12. S. Jalali Asadabadi, F. Kheradmand, "Ab initio prediction of magnetically dead layers in freestanding γ-Ce(111)", Journal Of Applied Physics 108, 073531 (2010).
13. S. Javanbakht, S. Jalali Asadabadi, "C atom endohedral doping effect on the bond lengths in the crystal structure of fcc-C60", I ranian Journal of Physics Research 10(4), 301-308 (2011).
14. M. Zarshenas, S. Jalali Asadabadi, "Theoretical study of alpha-U/W(110) thin films from density functional theory calculations: Structural, magnetic and electronic properties", Thin Solid Film 520, 2901-2908 (2012) (2012).
15. Mohsen Yazdanmehr, Saeid Jalali Asadabadi, Abolghasem Nourmohammadi, Majid Ghasemzadeh, and Mahmood Rezvanian, "Electronic structure and bandgap of γ-Al2O3 compound using mBJ exchange potential", Nanoscale Research Letters 7, 488 (2012).
16. Abolghasem Nourmohammadi, Saeid Jalali Asadabadi, Majid Gasemzadeh, Mohammad Hassan Yusefi, "Photoluminescence of Nanoporous Anodic Aluminum Oxide Membranes Prepared in Phosphoric Acid", Nanoscale Research Letters 7, 689 (2012).
17. 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, 181-184 (2013).
18. E. Ghasemikhah , S. Jalali Asadabadi, "Electronic properties of antiferromagnetic UBi2 metal by exact exchange for correlated electrons method" Iranian Journal of Physics Research 11, 4 (2012).
19. E. Ghasemikhah , S. Jalali Asadabadi, M. Dehghani,"Electric Field Gradients Calculations in UX2 (X=Bi, Sb) Compounds", Journal of Research on Many-Body Systems, 1, 21-23 (2011).
20. Zahid Ali, Iftikhar Ahmad, S. Jalali Asadabadi, "Comparison of band profiles and magnetic properties of the different phases" Computational Materials Science 67, 151–155 (2013).
21. Imad Khan, Iftikhar Ahmad, H.A. Rahnamaye Aliabad, S. Jalali Asadabadi, Zahid Ali, M. Maqbool, "Conversion of optically isotropic to

anisotropic CdS_xSe_{1-x} ($0 \leqslant x \leqslant 1$) alloy with S concentration", Computational Materials Science 77, 145-152 (2013).
22. Zahid Ali , Imad Khan, Iftikhar Ahmad, S. Naeem, H.A. Rahnamaye Aliabad, S. Jalali Asadabadi, D. Zhang, Physica B: Condensed Matter, " Comparison of the electronic band profiles and magneto-optic properties of cubic and orthorhombic $SrTbO_3$", 423, 16–20 (2013).
23. Zahid Ali, M. Shafiq, S. Jalali Asadabadi, H.A. Rahnamaye Aliabad, Imad Khan, Iftikhar Ahmad, "Magneto-electronic studies of anti-peroveskites NiNMn3 and ZnNMn3", Computational Materials Science, 81, 141-145 (2014).
24. 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, 88, 310-315 (2014).
25. M. Bilal, Banaras Khan, H. A. Rahnamaye Aliabad, Muhammad Maqbool, S. Jalali Asadabadi, Iftikhar Ahmad, "Thermoelectric properties of SbNCa3 and BiNCa3 for thermoelectric devices and alternative energy applications", Computer Physics Communications, 185, 1394 (2014).
26. M. Shafiq, Iftikhar Ahmad, and S. Jalali Asadabadi, "Theoretical studies of strongly correlated rare-earth intermetallics RIn3 and RSn3 (R=Sm, Eu, and Gd)", JOURNAL OF APPLIED PHYSICS 116, 103905 (2014).
27. M. Jamal, S. Jalali Asadabadi, Iftikhar Ahmad, H.A. Rahnamaye Aliabad, "Elastic constants of cubic crystals", Computational Materials Science 95, 592 (2014).
28. 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 (2015).
29. Banaras Khana, H.A. Rahnamaye Aliabad, N. Razghandi, M. Maqboold, S. Jalali Asadabadi, IftikharAhmad, "Structural and thermoelectric properties of pure and La, Y doped HoMnO3 for their use as alternative energy materials", Computer Physics Communications 187, 1 (2015).
30. M. Bilal, Saifullah, M. Shafiq, B. Khan, H.A. Rahnamaye Aliabad, S. Jalali Asadabadi, Iftikhar Ahmad" Antiperovskite compounds SbNSr3 and BiNSr3: Potential Candidates for Thermoelectric Renewable Energy Generators", Physics Letters A 379, 206 (2015).
31. Zahid Ali, Banaras Khan, Iftikhar Ahmad, Imad Khan, S. Jalali Asadabadi, "Magneto-electronic studies of the inverse-perovskite $(Eu_3O)In$", Journal of Magnetism and Magnetic Materials 381, 34-40 (2015).
32. M. Bilal, S. Jalali Asadabadi, Rashid Ahmad, Iftikhar Ahmad, "Electronic Properties of Antiperovskite Materials from State-of-the-Art Density Functional Theory", Journal of Chemistry 2015, 495131 (2015).
33. M. Bilal, Iftikhar Ahmad, S. Jalali Asadabadi, Rashid Ahmad, M. Maqbool, "Thermoelectric properties of Metallic Antiprovskites AXD3 (A=Ge, Sn, Pb, Al, Zn, Ga; X=N, C; D=Ca, Fe, Co", Electronic Materials Letters 11, 466 (2015).
34. Elham Gordanian, S. Jalali Asadabadi, Iftikhar Ahmad, S. Rahimi, M. Yazdani-Kachoei, "EFFECTS OF DANGLING BONDS

AND DIAMETER ON THE ELECTRONIC PROPERTIES OF InAs NANOWIRES", RSC Advances 5, 23320 (2015).
35. M. Shafiq, Iftikhar Ahmad, S. Jalali Asadabadi, "Mechanical properties and variation of SOC going from La to Nd in intermetallics RIn3 and RSn3 (R=La, Ce, Pr, Nd)", RSC Advances 5, 31496 (2015).
36. B. Khan, H. A. Rahnamye Aliabad, Saifullah, S. Jalali-Asadabadi, Iftikhar Ahmad, "Electronic Band Structures of Binary Skutterudites", Journal of Alloys and Compounds 647, 364 (2015).
37. Hadi Papi, Saeid Jalali-Asadabadi, Abolghasem Nourmohammadi, Iftikhar Ahmad, Javad Nematollahi, Mohsen Yazdanmehr, "Optical properties of ideal γ-Al2O3 and with oxygen point defects: An ab-initio study", RSC Advances 5, 55088 (2015).
38. Zahid Ali, Imad Khan, Iftikhar Ahmad, M. Salman Khan, S. Jalali-Asadabadi, "Theoretical studies of the paramagnetic perovskites MTaO3 (M=Ca, Sr and Ba)", Materials Chemistry and Physics 162, 308 (2015).
39. Zahid Ali, Abdul Sattar, S. Jalali-Asadabadi, Iftikhar Ahmad, "Theoretical studies of the osmium based perovskites AOsO3", Journal of Physics and Chemistry of Solids **86**, 114-121 (2015).
40. Esmaeil Ghasemikhah, Saeid Jalali-Asadabadi, Iftikhar Ahmad, Majid Yazdani-Kachoei, "Ab-initio studies of electric field gradients and magnetic properties of uranium dipnicties", RSC Advances **5**, 37592 (2015).
41. Saeid Jalali-Asadabadi, Esameil Ghasemikhah, Tarik Quahrani, Bromand Nourozi, Muhammad Bayat-Bayatani, Samaneh Javanbakht, Hossein Asghar Rahnamaye-Aliabad, Iftikhar Ahmad, Javad Nematollahi, Majid Yazdani-Kachoei, "Electronic Structure of Crystalline Buckyballs: fcc-C60", Journal of Electronic Materials, **45**, 339-348 (2016).
42. S. Ahmad, H. Vaizie, Hossein Asghar Rahnamaye-Aliabad, Rashid Ahmad, Imad Khan, Zahid Ali, S. Jalali-Asadabadi, Iftikhar Ahmad, Amir Abdullahkhan, "First-principles studies of pure and fluorine substituted alanines", International Journal of Modern Physics B, **30**, 1650079 (2016)**.**
43. M. Bilal, Iftikhar Ahmad, S. Jalali-Asadabadi, Rashid Ahmad, M. Shafiq, "DFT and post-DFT studies of metallic MXY 3-type compounds for low temperature TE applications", Solid State Communications **243**, 28-35 (2016).
44. Gul Rehman, M. Shafiq, Saifullah, Rashid Ahmad, S. Jalali-Asadabadi, M. Maqbool, Imad Khan, H. 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).
45. M. Yazdani-Kachoei, S. Jalali-Asadabadi, Iftikhar Ahmad, Kourosh Zarringhalam, "Pressure dependency of localization degree in heavy fermion CeIn3: A density functional theory analysis", Scientific Reports **6**, 31734 (2016).

46. Amin Khan, Zahid Ali, Imad Khan, S. Jalali-Asadabadi, Iftikhar Ahmad, "First-principle studies of the ternary palladates CaPd3O4 and SrPd3O4", Matter. Sci. **7**, 1861-1870 (2016).
47. 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).
48. 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 (AF4Sb12, A=Ca, Sr, and Ba)", Journal of Alloys and Compounds **694**, 253-260 (2017).
49. Sardar Ahmad, Rashid Ahamd, S. Jalali-Asadabadi, Zahid Ali, Iftikhar Ahmad, "First principle studies of electronic and magnetic properties of Lanthanide-Gold (RAu) binary Intermetallics", Journal of Magnetism and Magnetic Materials **422**, 458-463 (2017).
50. Mandana Safari, Zohreh Izadi, Jaafar Jalilian, Iftikhar Ahmad, S. Jalali-Asadabadi, "Metal mono-chalcogenides ZnX and CdX (X=S, Se and Te) monolayers: Chemical bond and optical interband transitions by first principles calculations", Physics Letters A **381**, 663-670 (2017), PDF.
51. Arash Boochani, Bromand Nowrozi, Jabar Khodadadi, Shahram Solaymani, S. Jalali-Asadabadi, "The Novel Graphene-Like Co2VAl (111): Case Study on Magnetoelectronic and Optical Properties by First Principles Calculations", Journal of Physical Chemistry C **121(7)**, 3978-3986 (2017).
52. Murad Ahmad, Gul Rehman, Liaqat Ali, M. Shafiq, Rashid Ahmad, Tahirzeb Khan, S. Jalali-Asadabadi, Muhammad, Maqbool, Iftikhar Ahmad, "Structural, electronic and optical properties of CsPbX3 (X=Cl, Br, I) for energy storage and hybrid solar cell applications", Journal of Alloys and compounds **705**, 828-839 (2017).
53. Imad Khan, Banaras Khan, Iftikhar Ahmad, Hossein Asghar Rahnamaye Aliabad, S. Jalali-Asadabadi, "Comparative study of thermoelectric properties of Co based filled Antimonide skutterudites with and without SOC effect", Computational Materials Science **131**, 308-314 (2017).
54. Imad Khan, Nasir Shehzad, Iftikhar Ahmad, Zahid Ali, S. Jalali-Asadabadi, "First-principle studies of the optoelectronic properties ofASnF3 (A=Na,K,RbandCs)", International Journal of Modern Physics B **31**, 1750148 (2017).
55. Rashid Iqbal, ZahidAli, S. Jalali-Asadabadi, IftikharAhmad, "Electron Correlation and Spin-Orbit Coupling Effects in Scandium Intermetallic Compounds ScTM (TM = Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag and Au)", International Journal of Modern Physics B **31**, 1750263 (2017).
56. Sajid Khan, Majid Yazdani-Kachoei, S. Jalali-Asadabadi, Iftikhar Ahmad, "Hyperfine Field, Electric Field Gradient, Quadrupole Coupling Constant and Magnetic Properties of Challenging Actinide Digallide", Physica B: Condensed Matter **526**, 102-109 (2017).

57. M. Shafiq, M. Yazdani-Kachoei, S. Jalali-Asadabadi, Iftikhar Ahmad, "Electric field gradient analysis of RIn3 and RSn3 compounds (R = La, Ce, Pr and Nd)", Intermetallics **91**, 95 (2017).
58. Rashid Iqbal, M. Bilal, S. Jalali-Asadabadi, H.A. Rahnamaye Aliabad, Iftikhar Ahmad, "Theoretical investigation of thermoelectric and elastic properties of intermetallic compounds ScTM (TM= Cu, Ag, Au and Pd)", In Press in International Journal of Modern Physics B **32**, 1850004 (2018).
59. Sajid Khan, Iftikhar Ahmad, M. Yazdani Kachoei, S. Jalali Asadabadi, M B Farooq, "Electronic and Magnetic structures as well as Magnetic HyperfineFields and Electric Field Gradients in UX3 (X=In, Tl, Pb) Intermetallic Compounds", Journal of Electronic Materials **47**, 1045-1058 (2018).
60. M. Jamal, M. Bilal, Iftikhar Ahmad, S. Jalali-Asadabadi, "IRelast package", Journal of Alloys and Compounds **735**, 569-579 (2018).
61. Sajid Khan, Majid Yazdani-Kachoei, S. Jalali-Asadabadi, Iftikhar Ahmad, "Theoretical studies of cubic AuCu3-type intermetallic actinide compounds NpPx3 (Px=Al, Ga, In)", Intermetallics **93**, 77-84 (2018).
62. Leila Mollabashi, Elham Sadeghi Kelishadi, Saeid Jalali-Asadabadi, "Crystal field and Ce^{3+} ion energy levels of $CeCl_3$ compound", Iranian Journal of Physics Research, **18**, 105-113 (2018).
63. Sardar Ahmad, M. Shafq, Rashid Ahmad, S. Jalali-Asadabadi, Iftikhar Ahmad, "Strongly correlated intermetallic rare-earth monoaurides (Ln-Au): ab-initio study", Journal of Rare Earths **36**, 1106-1111 (2018).
64. Muhammad Shafiq, Imad Khan, Ijaz Ahmad, Zahid Ali, S Jalali-Asadabadi, Iftikhar Ahmad, Amel Laref and Yasir Saeed, "Structural, Elastic and Thermal Properties of Lanthanide Monoantimonides", Advances in Materials Science and Engineering, **2**, Issue 1, 1-10 (2018).
65. Javad Nematollahi and Saeid Jalali-Asadabadi, "Microscopic Sources of Solid-States NMR Shielding in Titanate of Alkaline-Earth Perovskite Metals", Journal of Physical Chemistry C **122**, 20589-20601 (2018).
66. Reyhaneh Ebrahimi-Jaberi, Javad Nematollahi, Hadi Gharagoozloo, S. Jalali-Asadabadi, Morteza Jamal, "Elastic constants and their variation by pressure in cubic PbTiO3 compound using IRelast computational package within density functional theory", Iranian Journal of Physics Research, In Press, (2018).
67. M. Yazdanmehr, S. Jalali-Asadabadi, J. Nematollahi, A. Nourmohammadi, Iftikhar Ahmad, "Predictions of bandgap and subbands of γ−Al2O3 in presence of intrinsic point defects by DFT+TB-mBJ", Computational Condensed Matter **19**, e00379 (2019).
68. M. Yazdani-Kachoei, S. Jalali-Asadabadi, Negar Arianmehr, "Topological analysis of CeMIn5 (M = Co, Rh) electron charge

densities" Computational Materials Science **164**, 205-217 (2019).
69. M. Yazdani-Kachoei, S. Jalali-Asadabadi, " Thermoelectric properties of heavy fermion CeRhIn5 using density functional theory combined with semiclassical Boltzmann theory" RSC Advances **9**, 36182-36197 (2019).
70. M. Yazdani-Kachoei, S. Jalali-Asadabadi, "Topological analysis of electron density in half-Heusler ZrXBi (X = Co, Rh) compounds: A density functional theory study accompanied by Bader's quantum theory of atoms in molecules", In Press in Journal of Alloys and Compounds **828**, 154287 (2020).
71. Zeeshan Muhammd, Peitao Liu, Rashid Ahmad, S. Jalali Asadabadi, Cesare Franchini, Iftikhar Ahmad "Tunable Relativistic Quasiparticle Electronic and Excitonic Behavior of the $FAPb(I_{1-x}Br_x)_3$ Alloy", Physical Chemistry Chemical Physics **22**, 11943(2020).
72. Leila Mollabashi and S. Jalali-Asadabadi, "Crystal fields of lithium rare-earth tetrafluorides and multiplet splitting of the R+3 ions", Phys. Rev. B **102**, 045120 (2020).
73. Liaqat Ali, MuradAhmad, Muhammad Shafiq, Tahir Zeb, Rashid Ahmad, M. Maqbool, fIftikhar Ahmad, S. Jalali-Asadabadi, Bin Amin, "Theoretical studies of CsSnX3(X= Cl, Br and I) for energy storage and hybrid solar cell applications", Today Communications **25**, 101517 (2020).
74. M. Yazdani-Kachoei, S. Rahimi, R. Ebrahimi-Jaberi, J. Nematollahi, S. Jalali-Asadabadi, "Thermoelectric properties plus phonon and de Haas-van Alphen frequencies of hole/electron-doped CeIn 3", Scientific Reports **12**, 663 (2022).
75. Zeeshan Muhammad, Peitao Liu, Rashid Ahmad, Saeid Jalali-Asadabadi, Cesare Franchini, Iftikhar Ahmad, "Revealing the Quasiparticle Electronic and Excitonic Nature in Cubic, Tetragonal and Hexagonal Phases of FAPbI3", AIP Advances **12**, 025330 (2022).
76. Shahrbano Rahimi, Reyhaneh Ebrahimi-Jaberi, Farhad Jalali-Asadabadi, Leila Mollabashi, and S. Jalali-Asadabadi, "Influence of (Ba,F) multidoping on structural, magnetic, optical, and electrical properties as well as performance enhancement of multiferroic BiFeO3", Physical Review B **106**, 115205 (2022).
77. Muhammed Acikgoz, Leila Mollabashi, Shahrbano Rahimi, S. Jalali Asadabadi, and Czeslaw Rudowicz, "DFT computations combined with semiempirical modeling of variations with temperature of spectroscopic and magnetic properties of Gd3+-doped $PbTiO_3$", Physical Chemistry Chemical Physics **25**, 3986 (2023).
78. Arash Boochani, Moein Asshabi, Jabbar Khodadadi, Elmira Sartipi, Morteza Jamal, Jamshid Sabbagzadeh, Masoud Shahrokhi, Malieheh Amiri, Arash Yari, Shahram Solaymani, Amir hossein Sari, and Saeid Jalali-Asadabadi, "Co_2CrAl Heuslerene: Mechanical, Thermodynamic and Electronic Properties", Metals **13**, 582 (2013).
79. Reyhaneh Ebrahimi-Jaberi and S. Jalali-Asadabadi, "Anisotropic mechanical behavior and thermal attributes of antiferromagnetic UX2(X=P, As, Sb) materials: A density functional and elasticity

theories study", Materials Chemistry and Physics **312**, 128590 (2024).

80. Shahrbano Rahimi, S. Jalali-Asadabadi, Peter Blaha, Farhad Jalali-Asadabadi, "Nonzero spontaneous electric polarization in metals: Novel predictive methods and applications", Scientific Reports **14**, 672 (2024).
81. Leila Mollabashi, S. Jalali-Asadabadi, Czesław Rudowicz, Muhammed Acikgoz, Zahra Ghasemi-Dorcheh, Reyhaneh Ebrahimi-Jaberi, Mahdi Jalali-Asadabadi, Shahrbano Rahimi, and Farhad Jalali-Asadabadi, "Numerical study of the temperature-dependent magnetization and susceptibility of Tm^{3+} in $LiTmF_4$", Physical Review B **110**, 054440 (2024).
82. Reyhaneh Ebrahimi-Jaberi and Saeid Jalali-Asadabadi, "Elasticity and stability of $GdAl_2$ under pressure and temperature investigated using DFT+AI", Scientific Reports **15**, 15573 (2025).
83. Sharbano Rahimi and S. Jalali-Asadabadi, "Lone pair localization governs ferroelectric stability and excitonic properties in lead free halide perovskites", Scientific Reports **16**, 11409 (2026).
84. Leila Mollabashi, S. Jalali-Asadabadi, Shahrbano Rahimi, Czesław Rudowicz, Muhammed Acikgoz, "Crystal field induced defect compensation in Gd-doped $PbTiO_3$ preserving ferroelectricity and *f*-electron magnetism together with finite-temperature multifunctionality", Physical Review B **113**, 155125 (2026).

Conference and Workshop

1. S. Jalali Asadabadi, Numerical investigation of three rare-Earth valence-state in the compounds SmSn3-EuSn3-GdSn3, SPRING COLLEGE ON NUMERICAL METHODS IN ELECTRONIC STRUCTURE THEORY, 7 - 25 MAY 2001, ICTP, Miramare, Italy.
2. S. Jalali Asadabadi, H. Akbarzadeh and S. Cotteneer, Numerical Study of Three rare-Earth Valance-State in the compoundsSmSn3-EuSn3-GdSn3, Fifth Conference of Condensed Matter, Razi University of Kermanshah, winter (2001).
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9. S. Jalali Asadabadi, Electric Field Gradients within first principles of quantum mechanics calculations in CeIn3 , Seventh conference of condensed matter physics, University of Science and Technology, Tehran, Iran (2004).
10. S. Jalali Asadabadi, WIEN2k workshop (invited speaker to present a workshop on WIEN2k code), Seventh conference of condensed matter physics, University of Science and Technology, Tehran, Iran (2004).
11. S. Jalali Asadabadi, Properties predictions of solid states Ce-based compounds within ab initio calculations, Eight research week, University of Isfahan, 10-16 December (2005).
12. P. Rezaeian, S. Jalali Asadabadi, Elastic constants calculations of gamma-Ce, Annual Physics Conference, Lorestan University, Khoramabad (2005).
13. A. Fathi, S. Jalali Asadabadi, M. Goshtasbi Rad, H. Amini, Hyperfine interactions in USb2, Annual Physics Conference, Lorestan University, Khoramabad (2005).
14. S. Jalali Asadabadi, A preliminary introduction to WIEN2k code, Advanced workshop of WIEN2k code, Isfahan University of Technology, Isfahan, Iran (2006).
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16. S. Jalali Asadabadi, Brand new topics in WIEN2k code (II), Advanced workshop of WIEN2k code, Isfahan University of Technology, Isfahan, Iran (2006).
17. A. Fathi, Hyperfine Interactions in USb2, Advanced workshop of WIEN2k code, Isfahan University of Technology, Isfahan, Iran (2006).
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35. F. Vakili, S. Jalali Asadabadi, "Electric Field Gradients in GdAl2 Crystal", Shahid Chamran University of Ahvaz, Ahvaz, Iran (2009).
36. M. Dehghani, S. Jalali Asadabadi, "Evaluating the Properties of GdAl2 by Using of the Hybrid Exchange-Correlation Functionals Based on the Exact Exchange for Correlated Electrons (EECE) Method", Shahid Chamran University of Ahvaz, Ahvaz, Iran (2009).
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41. S. Pourmasoud, S. Jalali, "Investigation on Refraction, Reflectivity, and Extinction Coefficients in UPtGe Crystal", Annual Physics Conference of Iran, Bu-Ali Sina University, Hamadan, Iran, (2010).
42. S. Pourmasoud, S. Jalali Asadabadi, "Investigation on Structural, Electronic and Optical Properties of UPtGe Crystal", Annual Physics Conference of Iran, Bu-Ali Sina University, Hamadan, Iran, (2010).
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46. E. Gordanian, S. Jalali Asadabadi, M. Zarshenas, "Electronic and Structural Properties of Bulk InAs and the Role of Edge Atoms in Stability of its Nanowire within Density Functional Theory", 10th Condensed Matter Conference, Shiraz University, Shiraz, Iran (2011).

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Bonds in Poly-Alanine Alpha-Helix ", Annual Physics Conference of Iran, Yazd University, Yazd, Iran, 27-30 August (2012).

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63. B. Norozi, S. Jalali Asadabadi, "Structural and electronic properties of monolayer graphene doped Si by density functional theory calculations", Shahrood University of Technology, Shahrood, Iran (2013).
64. Z. Moseli, H. A. Rahnamaye Aliabad, S. Jalali Asadabadi, "Investigation of electrooptic properties of XRuO3(X=Ca, Sr) compounds", Shahrood University of Technology, Shahrood, Iran (2013).
65. N. Ardali, S. Jalali-Asadabadi, A. Rajabi, J. Nematollahi, F. Khoshhal, H. A. Rahnamaye-Aliabad, T. Ouahrani, "Investigation of topology of electron charge density in Fe2VAl Heusler-type compound", Computational Physics Conference of Iran, Shahid Rajaee Teacher Training University, Tehran, Iran, January 20-23 (2014) (30 Day to 2 Bahman 1392).
66. Sh. Shirkhar, S. Jalali-Asadabadi, J. Nematollahi, H. A. Rahnamaye-Aliabad, Iftikhar Ahmad, "Thermoelectric properties of BiNCa3", Computational Physics Conference of Iran, Shahid Rajaee Teacher Training University, Tehran, Iran, January 20-23 (2014) (30 Day to 2 Bahman 1392).
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69. Sh. Rahimi, S. Jalali-Asadabadi, M. Yazdani-Kachoei, J. Nematollahi, Oleg Rubel, "Calculation of spontaneous

polarization for beryllium oxide using modern polarization theory and Wannier functions", 20th Annual IASBS Meeting on Condensed Matter Physics & School on Soft Matter and Biological Physics, Institute for Advanced studies in Basic Sciences (IASBS), May 28-30, (2014) (7-9 Khordad 1393).

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73. J. Nematollahi, S. Jalali-Asadabadi, "Full potential nuclear magnetic resonance chemical shift of Fluoroperovskites AMF3 compounds with APW-based methods", 12th Condensed Matter Conference, Isfahan University of Technology, Isfahan, Iran (2015).
74. M. Yazdani-Kachoei, S. Jalali-Asadabadi, "First principle study of electronic structure and magnetic properties of CeIn3 compounds", 12th Condensed Matter Conference, Isfahan University of Technology, Isfahan, Iran (2015).
75. Majid Yazdani, Nilofar Hadaeghi, Sima Gheisarzadeh, Negar Ardali, Saeid Jalali-Asadabadi, "Invesitigation of magnetic, electronic, and topology of electron charge density of $CeRhIn_5$ compound", Annual Physics Conference of Iran, Ferdowsi University of Mashhad, Mashhad, Iran, 24-27 August (2015).
76. Nilofar Hadaeghi, Saeid Jalali-Asadabadi, Majid Yazdani-Kachoei, and Negar Aryamehr, "Investigation of electronic and topology of electron charge density in $CeIn_3$", Annual Physics Conference of Iran, Ferdowsi University of Mashhad, Mashhad, Iran, 24-27 August (2015).
77. Sima Gheisarzadeh, Saeid Jalali-Asadabadi, Majid Yazdani-Kachoei, and Javad Nematollahi, "Investigation of electronic and thermoelectric properties of $CePd_3$", Annual Physics Conference of Iran, Ferdowsi University of Mashhad, Mashhad, Iran, 24-27 August (2015).
78. Javad Nematollahi, Saeid Jalali-Asadabadi, "Structural, electronic, and optical properties of $KaTaO_3$: Ab initio investigation based on TB-mBJ exchange potential", Annual Physics Conference of Iran, Ferdowsi University of Mashhad, Mashhad, Iran, 24-27 August (2015).
79. Shahrebano Rahimi, Saeid Jalali-Asadabadi, Marzieh Pourshib, Zahra Ghasemi "De Hass-van Alphen Effect in UBi_2 Compound", Annual Physics Conference of Iran, Shiraz University, Iran, 22-25 August (2016).

80. Elham Sadeghi Kelishadi, Leila Mollabashi, Saeid Jalali-Asadabadi, Marzieh Pourshib, Zahra Ghasemi "Theoretical Determination of Crystal field Parameters of NdCl3 Using Wannier Functions", Annual Physics Conference of Iran, Shiraz University, Iran, 22-25 August (2016).
81. S. Jalali-Asadabadi, "Pressure Dependence of Localization Degree in Heavy Fermion $CeIn_3$: A Density Functional Theory Analysis", Autumn Meeting of the Physics Society of Iran, Department of Physics, University of Tehran, 10 December (2016).
82. Zahra Ghasemi Dorcheh, S. Jalali-Asadabadi, Leila Mollabashi, Elham Sadeghi Kelishadi, Shahrebano Rahimi, Majid Yazdani-Kachoei, Javad Nematollahi "Crystal Field Parameters Ho_2CoGa8 based on Wannier Functions", 13th Condensed Matter Conference, Shahid Rajaee Teacher Training University, Tehran, Iran (2017).
83. Marzieh Pourshib, S. Jalali-Asadabadi, Shahrebano Rahimi "Fermi Surface Investigation of UP_2 Compound", 13th Condensed Matter Conference, Shahid Rajaee Teacher Training University, Tehran, Iran (2017).
84. Javad Nematollahi, S. Jalali-Asadabadi, Zahra Ghasemi, Mehdi Fouladi Ardakani, "Full-Potential Nuclear Magnetic Resonance Chemical Shift Calculations of Titanium Perovskites Compounds based on APW Method", 13th Condensed Matter Conference, Shahid Rajaee Teacher Training University, Tehran, Iran (2017).
85. Zahra Ghasemi Dorcheh, Leila Mollabashi, S. Jalali-Asadabadi, "Determination of Crystal Fields Parameters of Gd3+ Ion in Tetragonal Structure using WANNIER Functions", Annual Physics Conference of Iran, Yazd University, Iran, 28-31 August (2017).
86. Reyhaneh Ebrahimi-Jaberi, Saeid Jalali-Asadabadi, Javad Nematollahi, Hadi Gharagoozloo, "Calculation of Elastic Constants in Cubic CdSe Compound within Density Functional Theory", Third Computational Physics Conference, Shahid Beheshti University, Tehran, Iran, 31 January to 1 February (2018).

Supervised Students

B.Sc. Thesis

- P. Rezaeian: Acoustic speeds calculations in gamma-Ce, University of Isfahan, Isfahan, Iran (Summer 2005).
- A. Armin: Optical properties of alpha-Ce, University of Isfahan, Isfahan, Iran (Summer 2005).
- H. Bolhassani, Investigation of Electronic Properties of Eu(001), (Summer 2010).
- Mahdi Jalali-Asadabadi, Machine Learning and its Applications in Density Functional Theory (Summer 2020).

M.Sc. Thesis

- A. Bochani, Structural and electronic properties of various phases of indium nitride (InN) semiconductor, University of Birjand, Birjand, Iran (Fall 2004).
- A. Fathi, Hyperfine interactions in USb2, University of Sistan and Balochestan, Zahedan, Iran (Winter 2006).

- M. Rafiee, Ab initio calculations to investigate electronic and structural properties of Pb/Si(111) interfaces, University of Isfahan, Isfahan, Iran (Summer 2007).
- F. Kheradmand, Surface magnetic moment calculation in α-Ce and γ-Ce, University of Isfahan, Isfahan, Iran (Summer 2008).
- S. Javanbakht, Electronic structure of fcc-C_{60} (Fall 2008).
- M. Sotodeh, Electric field gradients in Zr_3Fe, University of Isfahan, Isfahan, Iran (Fall 2008).
- A. Faghihi, Constraint LDA calculations to determine Hubbard U parameter, University of Isfahan, Isfahan, Iran (Fall 2008).
- M. Dehghani, Electronic structure of RAl2 and UX2 compounds within exact exchange for correlated electrons (EECE) method, (January 2010)
- F. Vakili, Calculation of electric field gradient in RAl_2 and RAl_3 (R = Rare Eraths), (Octobr 2010).
- M. Zarshenas, Surface properties of U/W(110) thin films, (October 2010).
- S. Pourmasoud, Optical properties of UPtGe compound, (November 2010).
- E. Gordanian, "Investigation of structural and electronic properties of InAs bulk and its nanowires in zincblende and wurtzite phases", (June 2011).
- E. Ghasemikhah, "Magnetic Properties and Electric Field Gradients Calculations in Antiferromagnetic States of UX2(X=P, Sb, Bi) within LDA+U and Exact Exchange for Correlated Electrons (EECE)", (July 2011).
- M. Ghasemzadeh, "Effect of Anodizing Parameters on the Bandgap of Nanoporous Anodic Aluminum Oxide Membranes", (Ocobr 2011).
- B. Norozi, "Investigation of Strain, distortion and dopping effects on the Structural and Electronic Properties of Graphene", (March 2012).
- M. Bayat Bayatani, "Topology of Charge Density in Pristine and Doped fcc-C60 Crystal", (March 2012).
- M. Rezvanian, "Study of hydrogen bonds in polyalanine chains in the alpha helical nanostructure by employing density functional theory", (November 2012).
- M. Yazdanmehr, "Experimental and theoretical investigations of Bulk structure and nanosurface structure of aluminum oxide in gamma phase (gamma-Al2O3)", (2012).
- S. Reesy, "Structural, electronic and thermodynamic properties of formamide under hydrostatic pressure using density functional theory", (November 9, 2013).
- H. Papi, "Surface and optical properties of γ-Al_2O_3 thin films from experimental measurements and ab initio DFT calculations", (Octobr, 2013).
- F. Khoshhal-Dehdar, "Electronic structure, magnetic properties and electric field gradients in bulk and nano-thin films of rare earth compounds", January 2014.
- Sh. Rahimi, "Study of Berry phase, Born effective charge and spontaneous polarization in III-V, II-V, ABO3 groups and InAs nanowire within density functional theory", September 2014.
- Sh. Shirkhar, "Effects of chemical pressure on the transport properties of $Fe_2V_{1-x}nb_xAl$ and CeM_xIn_{3-x}, $CeRhM_xIn_{5-x}$ (M=Cd, Sn) and $CePt_2In_7$ compounds", November 2014.

Ph.D. Students

- N. Ardali (Arianmehr), "Investigation of topology of charge density in Fe2V1-xNbxAl Heusler compounds and CeMxIn3-x, CeRhMxIn5-x, CePt2MxIn7-x (M=Cd, Sn) 4f-electron systems", September 2014.
- S. Gheisarzadeh, "Transport Properties and Charge Density Topological Analysis of Some Lanthanide (Rare-Earth) based Compounds", (February 2016).
- N. Hadaeghi, "Spontaneous polarization and topological Charge Density Analysis of Some of the Lanthanide based Compounds", (February 2016).
- Elham Sadeghi, "Calculation of crystal field parameters for lanthanide based compounds RCl_3 (R=Ce, Pr, Nd)", (November 2016).
- Mehdi Fouladi, "Study of chemical shielding tensor of PbTe compound in the presence of Sn and Ge impurities", September 2017.
- Zahra Ghasemi Dorche, "Crystal Field Parameters and electronic properties for lanthanide compounds", February 2018.
- Marzieh Pourshib, "Determination of Fermi surfaces and De Hass-van Alphen frequencies in UX2(X=P, As, Sb) compounds", May 2018.
- Hadi Gharaghoozloo, "Valence determination of lanthanide compounds using the of their structural and electronic properties", September 2019.

Iranian Ph.D. Thesis

- Majid Yazdani-Kachoei, "Electronic, magnetic, transport properties, and hyperfine interactions of CeM_xIn_{3-x}, $CeRhM_xIn_{5-x}$, $CePt_2M_xIn_{7-x}$ (M=Cd, Sn) compounds", February 2018.
- Javad Nematollahi, "Ab initio calculations of structural and electronic properties as well as nuclear magnetic resonance chemical shielding tensors in solid-state crystals", January 2019.
- Leila MMollabashi, "Crystal fields of lithium rare-earth tetrafluorides and multiplet splitting of the R+3 ions
- " 2020.
- Shahrbano Rahimi, "Influence of (Ba,F) multidoping on structural, magnetic, optical, and electrical properties as well as performance enhancement of multiferroic BiFeO3", 2023.
- Reyhaneh Ebrahimi-Jaberi, "Dynamical mean field theory to study strongly correlated materials", 2024.
- Atefeh Marasi, Working.
- Zahra Ghasemi-Dorcheh, Working.
- Ali Shahnazari, Working.
- Mahdi Jalali-Asadabadi, Working.

Pakistani Ph.D. Thesis

- Muhammad Shafig, "Theoretical studies of strongly correlated lanthanide intermetallics LnX_3 (X=In, Sn)", February 2015.

- Sajid Khan, "EFG AND MAGNETIC STUDIES OF ACTINIDE–POST TRANSITION METALS", 2018.
- Rashid Iqbal, "THEORETICAL STUDIES OF LANTHANIDE TRANSITION METAL INTERMETALLICS IN CsCl-STRUCTURE", 2018.
- Fawad Kjan, "FIRST PRINCIPLE INVESTIGATION OF ELECTRONIC STRUCTURE AND THERMOELECTRIC PROPERTIES OF LAYERED TRANSITION METAL DICHALCOGENIDES", 2020.
- Saif Ullah, "PHYSICAL PROPERTIES AND CORRELATION EFFECTS OF TRANSITION METAL PEROVSKITE OXIDES", 2020.
- Zeeshan Muhammad, "ORGANIC-INORGANIC HYBRID PEROVSKITE SOLAR CELL MATERIALS: DFT STUDIES", 20201.

Postdoctoral Researchers

Postdoc Researchers

- Majid Yazdani-Kachoei, "Thermoelectric properties and topological analysis of half-Heusler ZrXBi (X~=~Co, Rh) compounds", 2020.
- Leila Mollabashi, "Crystal Field Theory", 2023.
- Shahrbano Rahimi, Working.

Membership & Scientific Activities

❖ Member of Physics Society of Iran (PSI)	2010-Now
❖ Member of American Physics Society (APS)	2008-2012
❖ Text Editor of Iranian Journal of Research Physics (IJRP), Isfahan University of Technology, Isfahan, Iran	1998-Now 2012-2017 1998-2003
❖ Member of Editorial Board of Journal of Physics-Bioinfo Publications	2012
❖ Member of Promoter Committee of Computational Physics Branch (CPB) of Physics Society of Iran (PSI)	2013
❖ Member of Computational Physics Branch (CPB) of Physics Society of Iran	27-30 August
❖ Member of Condensed Matter Physics Branch (CMPB) of Physics Society of Iran (PSI)	2012
❖ Member of Scientific Committee of Annual Physics Conference of Iran, Yazd University, Yazd, Iran	2012
❖ Member of Advisory Board of International Workshop on Materials Modeling and Simulations (IWMMS)	2010
❖ Member of Scientific Committee of Tenth Condensed Matter Conference, Shriaz university, Shiraz	Spring 2011
❖ Director and Organizer of Advanced Workshop on All Electron Density Functional Theory Based Calculations	
❖ Director and Organizer of Fall School on Density Functional Theory	Fall 2008
❖ Member of Organizers of Advanced Workshop on WIEN2k Computational Package	2005 2002

- Member of Organizers of Regional Workshop on Computational Condensed Matter—WIEN2k Advanced Workshop — 2001
- Member of Organizers of Preliminary Workshop on Computational Condensed Matter--Introduction to WIEN2k — Winter 2014
- Member of Scientific Committee of the first Computational Physics Conference — Winter 2015
- Director of Scientific Committee of 12th Condensed Matter Conference of the Physics Society of Iran — Winter 2017
- Member of Scientific Committee of 13th Condensed Matter Conference of the Physics Society of Iran — Fall 2018
- Member of Organizers and Scientific Directors of 2ND INTERNATIONAL CONFERENCE AND EXHIBITION ON NANOTECHNOLOGY (ICENT), San Diego, USA, November 19-21 — Winter 2019
- Member of Scientific Committee of the 14th Condensed Matter of Physics Society of Iran — Summer 2019
- Member of Scientific Committee of Annual Physics Conference of Iran — Winter 2020
- Member of Scientific Committee of the fourth Computational Physics of Physics Society of Iran — Summer 2014
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Favorite Sport

- Taekwondo, Black Belt, Dan 2

Old Extra Activities

- Teaching Physics and Mathematics in Center for Brilliant Students, Alameieh Heli, Tehran, Iran — 1990-91
- Developing Computer Softwares in Hoshiarpardaz Company, Tehran, Iran — 1993-95
- Teaching Computer Programing Languages in ISIRAN INSTITUTE, Tehran, Iran — 1994-95
- Working in High Power Fast Pulse Laser Laboratory, Leaser Research Center, Tehran, Iran — 1995-96