

Curriculum vita

Associate professor in Solid state physics and Nanophysics

Personal

Name: Tayebeh Movlarooy

Nationality: Iranian

Place of birth: Fariman, Iran
Date of birth: 16 Sep, 1976

Gender: Female

Position: Associate professor in Solid state physics and Nanophysics

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DEGREE

Ph.D: Solid state physics, *Thesis: Theoretical calculations of electronic and optical properties of SWCNTs and Peapods, under the supervision of Professors: S. M. Hosseini, A. Kompany and Claudia Ambrosch-Draxl,* Ferdowsi University of Mashhad, Mashhad, Iran (2005-2010)

M.Sc: Solid state physics, Ferdowsi University of Mashhad, Mashhad, Iran (2002-2005)

B.Sc: physics, Ferdowsi University of Mashhad, Mashhad, Iran (1998-2002)

PROMOTION

Assistant Professor in Solid state physics and Nanophysics, 2010-2018.

Associate professor in Solid state physics and Nanophysics, 2018 – present

Teaching Experiences

- ❖ Numerical Modeling and Simulation in Condensed Matter, Density functional theory, Numerical physics, Solid state physics, Advanced Solid state physics, Computational physics, Nanophysics, Computer, Fortran programming, Analytical Mechanics, Quantum mechanics, Electromagnetic, Many Body Physics and Basic physics in *Shahrood University of Technology, Shahrood, IRAN*.
- ❖ Basic Physics, physics labs, Electromagnetic in *Ferdowsi University of Mashhad, Mashad, IRAN*.
- ❖ Basic Physics, Electromagnetic and Quantum mechanics in *Payam Noor University of Mashhad, Mashhad, IRAN*.

Principal Fields of Interest

- ❖ Computational condensed matter physics and Computational Material Science based on the density functional theory (DFT).
- Simulation and Modeling of bulk materials, surfaces and Nanostructures.
- Simulation and Modeling of Nano sensors, solar cells, spintronic devices and etc.
- ❖ High performance computing on the electronic structure and physical properties of nanostructures.
- Nanomaterials
- ❖ Investigation of a broad range of properties such as:

Structural and electronic properties.

Magnetic properties.
Optical properties.
Transport Properties.
Spintronics.

Computer Skills

- ❖ DFT Packages like: Wien2k, Quantum-ESPRESSO, and Siesta.
- ❖ Languages: Fortran,.
- Operating Systems: Linux, Windows.
- Microsoft office, Origin, Word, Powerpoint.
- ❖ Simulation packages (Gauss View, ATK (Atomistix Tool Kit)).
- ❖ Familiar with computational approaches like as DFT, NEGF

Visits:

Chair of Atomistic Modelling and Design of Materials, University of Leoben, Leoben, Austria, for one year (2008), under Supervision of Prof. Claudia Ambrosch-Draxl.

Awards:

PhD. Scholarship, Ministry of Science, Research, and Technology, Iran (2005-2010).

Study opportunity scholarship, Ministry of Science, Research, and Technology, Iran, 2008.

Guest Researcher Scholarship, Chair of Atomistic Modelling and Design of Materials, University of Leoben, Leoben, Austria, 2008.

Top Researcher: The Top researcher of the Shahrood University of Technology and the Top researcher of the Semnan province in 2023.

Workshops activities

- ➤ National workshop on Wien2k, 2006.
- National workshop on Quantum espresso code (PWSCF), 2008.
- NaPhoD-Summerschool, Porto Conte Ricerche, Sardinia, Italy, 15-20 September, 2008.
- ➤ Workshop on Trends in nanoscience: theory, experiment, technology, Sibiu, Romania, 23-30 Aug, 2009.
- ➤ 4th HPC workshop (HPC4), 2011, IPM, IRAN.
- ➤ 9th SESAME Users' Meeting, Amman, Jordan, 12 16 November 2011.
- ➤ 10th SESAME Users' Meeting, Amman, Jordan, 7 9 November 2012.

Supervisor of Ph.D and M. Sc Theses:

Supervisor of 8 Ph.D and 24 M. Sc Theses.

The M.Sc and Ph.D theses which are running now under my supervision are as follows:

1. Akram Malek, Ph.D Student, "DFT study of Phosphorene as a promising biosensor for the detection of lung cancer exhalation biomarkers" Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor].

- 2. Hamed Samandari, Ph.D Student, "study of structural and electronic properties of graphyne nanostructures using density functional theory" Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor].
- 3. Azadeh Mohammadkhani, Ph.D Student, Shahrood University Of Technology, Tayebeh Movlarooy [Supervisor].
- 4. Aliasghar Moradipur, Ph.D Student, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor].

The M.Sc and Ph.D theses which have done under my supervision are as follows:

- 1. Adeleh Vatankhahan (2021), "Study of transport properties of borophene by non-equilibrium Green functional and DFT method" Ph.D Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor],
- 2. Mhboobeh Amiri Fadradi (2023), "The physical properties of gas molecules adsorbed on single-walled BN naontubes" Ph.D Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor].
- 3. Sorour Faramarzi (2023), "Investigation of the structures and physical properties of borophene as a promising anode material for Ion batteries" Ph.D Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor].
- 4. Tahmineh Khademi (2023), "Analysis and simulation of electron and optical properties of absorber layer of lead free hybrid perovskite solar cells based on SnGe and BiCu", Ph.D Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor].
- 5. Azadeh Mohammadkhani (2023), "Study of adsorption of gas molecules on borophene nanoribbons for sensor applications" Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor],
- 6. Mohadese Anavi (2021), "Study of optical and electronic properties of absorbing laxyers of bismuth-baxsed perovskite solar cells", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor],
- 7. Akram Nooranbjar (2020), "Simulation of gas nanosensors baxsed on Graphyne nanosheets", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor],
- 8. Parian Jamei (2020), "Theoretical and Experimental Study of Sensing Properties of Tin Oxide Nanostructures (SnO2)", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy, Hamid Haratizadeh[Supervisor],
- 9. Sadegh Nik bakhtian (2019), "Investigation of stability and electronic stracture of double-walled Gallium-Arsenide (GaAs) nanotubes by density functional

- theory", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor],
- 10. Raaziyeh Hosseini (2019), "Investigation of stability and electronic properties of double-walled AlN nanotubes ", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor], Saeid Hessami Pilehrood[Advisor]
- 11. Asma Sedaghatparvar (2019), "Simulation of Gas Sensors baxsed on Single Walled Zinc Oxide Nanotubes", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor], Saeid Hessami Pilehrood[Advisor]
- 12. Mehrzad Beiranvand (2018), "Investigation of electronic and magnetic properties of transition mextals doped AlN nanosheets for the application in spintronic devices", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor], Fatemeh Badieian Baghsiyahi[Advisor]
- 13. Zahra Afshoon (2018), "Study of electronic and magnetic properties of silicon carbide nanotube filled by transition mextals", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor],
- 14. Vajiheh Allahverdinejad sarab (2018), "Study of stability and electronic properties of pure and doped double-walled ZnO nanotubes", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor],
- 15. Mohamad reza Keyghobadi moghaddam (2018), "Study of stability and electronic properties of double-walled Gallium-nitride nanotubes", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor], Saeid Hessami Pilehrood[Advisor]
- 16. Saberi Aliabadi Soheila (2018), "Simulation of Gas Nanosensors baxsed on Zinc Oxide Nanosheets", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor], Saeid Hessami Pilehrood[Advisor]
- 17. Narges Arabhajji (2017), "Density functional theory Study of electronic and optical properties of GaN and its", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor], Fatemeh Badieian Baghsiahi[Advisor]
- 18. Parvin Zanganeh (2016), "Transport properties of grapheme nanoribbons: a DFT investigation", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor],
- 19. Mahboobeh Amiri Fadardi (2016), "Study of The physical properties of gas molecules adsorbed on single-walled BN naontubes", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor],
- 20. akram malek (2016), "Investigation of electronic and magnetic properties of transition mextals doped BN nanosheets", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor], Saeid Hessami Pilehrood[Advisor]

- 21. Babak Minaie (2016), "Investigation of electronic properties and stability of double-walled BN nanotubes ", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor],
- 22. Mehdi Motaharinejad (2015), "Study of stability and electronic properties of double-walled silicon carbide nanotubes", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy, Saeid Hessami Pilehrood[Supervisor],
- 23. Mohammadreza Fallah Hamidabadi (2015), "Study of structural and magnetic properties of transition mextals encapsulated inside Silicon Nanotubes", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy, Saeid Hessami Pilehrood[Supervisor],
- 24. Farshid Enayati Sangesereki (2015), "First principles study of transport properties of oligothiophenes", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor], Raheleh Pilevar Shahri[Advisor]
- 25. Mohammad Afzali (2015), "Study of electronic and transport properties of GaN nanoribbons by means of density functional theory (DFT)", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor], Saeid Hessami Pilehrood[Advisor]
- 26. Bahareh Asgharpoor (2015), "Scattering in Quantum Wires under Electromagnetic Radiation", Msc Thesis, Shahrood University Of Technology, Saeid Hessami Pilehrood, Tayebeh Movlarooy[Supervisor],
- 27. Reza Fathi (2015), "Study of electronic and magnetic properties of GaAs nanotubes by means of density functional theory (DFT) approach", Msc Thesis, Shahrood University Of Technology, Tayebeh Movlarooy[Supervisor],
- 28. Mostafa Shabani (2014), "Study of Electronic and Magnetic properties of Transition mextal doped GaN nanotubes by means of Density Functional Theory approach ", Msc Thesis, Shahrood University Of Technology, Saeid Hessami Pilehrood, Tayebeh Movlarooy[Supervisor],

Participating in projects as a project leader

1. Study of physical properties of one dimensional ZnO nanostructures doped with transition metal for spintronic application, (2013-2014).

Paper based on this project:

- T Movlarooy, "Transition metals doped and encapsulated ZnO nanotubes: Good materials for the spintronic applications", Journal of Magnetism and Magnetic Materials 441, 139-148. (2017).
- 2. Study of electronic properties and quantum confinement effect in ZnO nanotubes and nano wires, (2015)

Paper based on this project:

- T Movlarooy, "Study of quantum confinement effects in ZnO nanostructures", Materials Research Express 5 (3), 035032. (2018).
- 3. Study of physical properties of carbon, boron nitride and silicon carbide structures of (2,2) armchair nanotube by using DFT,(2011)

Paper based on this project:

DV Fakhrabad, T Movlarooy, N Shahtahmassebi, Density functional theory study of ultrasmall diameter (2, 2) boron nitride, silicon carbide, and carbon nanotubes, physica status solidi (b) 249 (5), 1027-1032. (2012).

4. Studying the electronic and magnetic properties of chromium phosphor nanoribbons for spintronic applications, (2023)

Paper based on this project:

Adeleh Vatankhahan, TayebehMovlarooy, "Ferromagnetic Half-metal with High Curie temperature in CrP nanoribbons: good material for electronic and spintronic applications", Physical Chemistry Chemical Physics 25 (35), 24155-24162, (2023).

Publications and Symposium Proceedings

Published ISI Papers:

- 1. SM Hosseini, T Movlarooy, A Kompany, (2007), "First-principle calculations of the cohesive energy and the electronic properties of PbTiO3", Physica B: Condensed Matter 391 (2), 316-321.
- 2. T Movlarooy, A Kompany, SM Hosseini, N Shahtahmasebi, (2010) "Optical absorption and electron energy loss spectra of single-walled carbon nanotubes", Computational Materials Science 49 (3), 450-456.
- 3. T Movlarooy, MA Fadradi, (2018), "Adsorption of cyanogen chloride on the surface of boron nitride nanotubes for CNCl sensing", Chemical Physics Letters 700, 7-14. https://doi.org/10.1016/j.cplett.2018.04.001
- 4. T Movlarooy, (2017), "Transition metals doped and encapsulated ZnO nanotubes: Good materials for the spintronic applications", Journal of Magnetism and Magnetic Materials 441, 139-148.
- 5. N Ghajari, A Kompany, T Movlarooy, F Roozban, M Majidiyan,(2013) "Synthesis, experimental and theoretical investigations of Zn1- xCuxO nanopowders", Journal of magnetism and magnetic materials 325, 42-46
- 6. DV Fakhrabad, T Movlarooy, N Shahtahmassebi,(2012)," Density functional theory study of ultrasmall diameter (2, 2) boron nitride, silicon carbide, and carbon nanotubes", physica status solidi (b) 249 (5), 1027-1032
- 7. MA Fadradi, T Movlarooy, (2018), "Ab initio study of adsorption of CO on BNNTs: For gas nanosensor applications", Materials Chemistry and Physics 215, 360-367. https://doi.org/10.1016/j.matchemphys.2018.04.102
- 8. T Movlarooy, (2013)," The effect of intraband transitions on the optical spectra of metallic carbon nanotubes", Chinese Physics Letters 30 (7), 077301

- 9. T Movlarooy, P Zanganeh,(2019)," Spin transport properties of armchair graphene nanoribbons doped with Fe and B atoms", Materials Science and Engineering: B 243, 167-174. DOI:10.1016/j.mseb.2019.04.014
- 10. T Movlarooy, (2018)," Study of quantum confinement effects in ZnO nanostructures", Materials Research Express 5 (3), 035032
- 11. T Movlarooy, SM Hosseini, A Kompany, N Shahtahmasebi, (2011), "Ab initio calculations of electronic structure and optical spectra of (13-0) carbon nanotube", International Journal of Nanoscience 10 (04n05), 587-590
- 12. SM Hosseini, T Movlarooy, A Kompany, (2005), "First-principles study of the optical properties of PbTiO3", The European Physical Journal B46 (4).
- 13. T Movlarooy, SM Hosseini, A Kompany, N Shahtahmasebi, (2010)," Ab initio calculations of optical spectra of a chiral (4,1) carbon nanotube", physica status solidi (b) 247 (7), 1814-1821
- 14. T Movlarooy, B Minaie, (2018), "First principles study of structural and electronic properties of BNNTs", Journal of Computational Electronics 17 (4), 1441-1449
- 15. T Movlarooy, F Enayati, R Pilevarshahri, (2019), "Molecular junction of n-thiophenes sandwiched between two Au (111) electrodes", Molecular Physics 117 (1), 6-10.
- 16. T Movlarooy, (2014), "Polythiophene encapsulated inside (13, 0) CNT: A nanohybrid system", Chinese Physics B 23 (6), 066201.
- 17. A Vatankhahan, T Movlarooy, (2021), "The effect of edges hydrogenation and adsorption of Co and Mn atoms on spin transport properties of borophene Nanoribbons", Materials Science and Engineering: B 273, 115391. doi:10.1016/j.mseb.2021.115391
- 18. A Malek, T Movlarooy, SH Pilehrood, (2019), "Ground-State Magnetic Phase in Transition-Metal-Doped Boron Nitride Nanosheet With (5, 0) Chirality", IEEE Magnetics Letters 10, 1-4. DOI: 10.1109/LMAG.2019.2951085
- 19. R Fathi, T Movlarooy, (2018)," Electronic and structural properties of semiconductor GaAs nanotubes", Journal of Electronic Materials 47 (12), 7358-7364
- 20. M Beyranvand, T Movlarooy, FB Baghsiyahi, (2020), "Magnetic phase stability of transition metals doped (4, 4) AlN nanosheet", Journal of Magnetism and Magnetic Materials 497, 166028. https://doi.org/10.1016/j.jmmm.2019.166028
- 21. R Fathi, T Movlarooy, (2019), "Magnetic properties of zigzag (0, 9) GaAs nanotube doped with 3d transition metals", Iranian Journal of Physics Research 16 (1), 35-44
- 22. A Vatankhahan, T Movlarooy, (2020), "Ab Initio Study of Transition Metal Adsorption on a Borophene Nanosheet", IEEE Magnetics Letters 11, 1-5
- 23. T Movlarooy, M Motaharinezhad, S Hessami Pilehrood, (2019)," Study of the stability and interwall distance of (6, 0)@(n, 0) double-walled silicon carbide nanotubes by the vdW-DFT method", Iranian Journal of Physics Research 18 (4), 705-711
- 24. N. Ghajari, AN Kompany, T Movlarooy, F Roozban, M Majidiyan, (2013), "Synthesis, experimental and theoretical investigations of Zn1-xCuxO nanopowders", Journal of Magnetism and Magnetic Materials 325, 42-46.
- 25. A Vatankhahan, T Movlarooy, (2022)," Modulating spintronic properties of Nitrogen passivated borophene nanoribbons", Materials Science and Engineering: B 281, 115744. https://doi.org/10.1016/j.mseb.2022.115744
- 26. R Hosseini, T Movlarooy, A Vatankhahan, (2022), "Electronic structures and stability of double-walled armchair and zigzag AlN nanotubes", Materials Science and Engineering: B 286, 115973.

- 27. V Allahverdinejad sarab, T Movlarooy, (2022), "Structural and electronic properties of double-walled zigzag and armchair Zinc oxide nanotubes", Chinese Journal of Physics, https://doi.org/10.1016/j.cjph.2022.08.004.
- 28. A. Malek, T. Movlarooy, S. Hessami Pilehrood," Transition metals doped (3,3) armchair boron nitride nanosheet as dilute magnetic semiconductors materials for the spintronic application", Int. J. Quantum Chem. 2022, e27070. https://doi.org/10.1002/qua.27070.
- 29. M. Shabani, T. Movlarooy, S. Hessami Pilehrood, "Modulating spintronic properties of transition metals doped GaN nanotubes with high Curie temperature", Int. J. Quantum Chem. <u>Volume123</u>, <u>Issue9</u>, 2023, e27079. https://doi.org/10.1002/qua.27079.
- 30. Parvin Zanganeh, Tayebeh Movlarooy, (2015), "Investigation of structural and magnetic properties of graphene nanoribbons doped with Fe atoms", Journal of Research on Many-body Systems, 10.22055/jrmbs.2016.12481.
- 31. Tayebeh Movlarooy, (2018) Nanomeghyas, Volume:4 Issue: 4, Pages:295 301. magiran.com/p1816365.
- 32. M Motaharinejad, T Movlarooy, S Hessami Pilehrood, (2023), "Electronic structures and stability of double-walled armchair (n, n)@(m, m) SiC nanotubes", Journal of Computational Electronic, (2023), https://doi.org/10.1007/s10825-023-02012-0.
- 33. Razieh Hosseini, Tayebeh Movlarooy, Adeleh Vatankhahan, "Tuning electronic and structural properties of single wall AlN nanotubes", Modern Physics Letters B, Accepted, (2023).
- 34. Babak Minaie, Tayebeh Movlarooy, "Ab initio study of structural properties and inter-wall distances of double-walled BN nanotubes", Modern Physics Letters B. (2023) https://doi.org/10.1142/S0217984923500240.
- 35. Sadegh Nikbakhtian, Tayebeh Movlarooy, "Tuning inter-wall spacing and structural properties of double-walled Gallium Arsenide nanotubes", Int. J. Quantum Chem. Accepted (2023). https://doi.org/10.1002/qua.27105
- 36. Mohamadreza Keyghobadi-moghaddam, Tayebeh Movlarooy, "Tuning structural properties and inter-wall spacing of double-walled GaN nanotubes", physica status solidi a, Volume220, Issue7, 2200758, (2023). https://doi.org/10.1002/pssa.202200758
- 37. Mehrzad Beyranvand, Tayebeh Movlarooy, Fatemeh Badieian Baghsiyahi," Ab initio study of electronic and magnetic properties of Zigzag and Armchair AlN Nanosheets", Physica E, Volume 150, June 2023, 115670.
- 38. Zahra Afshoon, Tayebeh Movlarooy,"Tuning structural and electronic properties of single-walled SiC nanotubes ", Silicon, (2023). https://doi.org/10.1007/s12633-023-02314-9. https://doi.org/10.1007/s12633-023-02314-9.
- 39. Mahboobeh Amiri Fadardi, Tayebeh Movlarooy," Simulation of NOx and COx Gas Sensor Based on Pristine Armchair Stanene Nanoribbon", Advanced Theory and Simulations, Volume6, Issue11, (2023), https://doi.org/10.1002/adts.202200925
- 40. Sorour Faramarzi and Tayebeh Movlarooy, "Tuning structural and electronic properties of β 12-Borophene/Graphene heterostructure", Modern Physics Letters B, 2350051, (2023).
- 41. Tahmineh Khademi, Tayebeh Movlarooy, "Exploring Optical and Electronic Properties of 2D Lead-Free Hybrid Perovskites Based on Sn-Ge for photovoltaic applications", IEEE Journal of Photovoltaics, (2023).
- 42. Tahmineh Khademi, Tayebeh Movlarooy, "Investigating the Effect of Halogens on the Electronic and Optical Properties of Lead-Free Double Halide Perovskites Based on Cu-Bi", International Journal of Quantum Chemistry 123 (16), e27139, (2023).

- 43. Adeleh Vatankhahan, TayebehMovlarooy, "Ferromagnetic Half-metal with High Curie temperature in CrP nanoribbons: good material for electronic and spintronic applications", Physical Chemistry Chemical Physics 25 (35), 24155-24162, (2023).
- 44. Adeleh Vatankhahan, TayebehMovlarooy, "DFT study of High-Curie-temperature ferromagnetism in α-borophene nanoribbons for spintronic applications", Advanced Theory and Simulations 6 (11), 2200925, (2023).
- 45. Parvin Zanganeh, Tayebeh Movlarooy, "Investigating the electronic and magnetic properties of graphene nanoribbons using density functional theory", Nanomeghyas, Volume 10, Issue 2, August 2023, Pages 48-53, (2023).
- 46. Tahmineh Khademi, Tayebeh Movlarooy, "the effect of cations in electronic, and optical properties of 3D lead-free halide perovskites based on Sn-Ge", Modern Physics Letters B, 2350123, (2023).
- 47. M. Shabani, T. Movlarooy, S. Hessami Pilehrood, "DFT study of electronic and structural properties of single-walled Gallium Nitride nanotubes", International Journal of Quantum Chemistry 123 (17), e27141, (2023).
- 48. A. Mohamadkhani and T. Movlarooy, "Gas Molecules Adsorption on $\beta_{1\ 2}$ Borophene Nanoribbons and Nanosheets for the Gas Sensor Applications," in *IEEE Sensors Journal*, vol. 24, no. 7, pp. 10270-10276, 1 April1, 2024, doi: 10.1109/JSEN.2024.3363872.
- 49. Faramarzi, Sorour; Movlarooy, Tayebeh, "Catalyzing Energy Storage: Graphene-Borophene Heterostructure as a High-Performance Anode Material for Li-Ion Batteries", ACS Applied Materials & Interfaces (2024).
- 50. Mahboobeh Amiri Fadardi, et al, "study of Carbon monoxide adsorption on B-N doped hydrogenated Sn nanoribbons towards nanosensor applications", Chinese Journal of Physics, 90, (2024) 31-41. https://doi.org/10.1016/j.cjph.2024.04.043
- 51. T Movlarooy, A Nooranbjar, "Gas molecules adsorption on the α -Graphyne nanosheet for the sensor applications", Diamond and Related Materials 148, 111471
- 52. T Movlarooy, A Nooranbjar, "Study of carbon monoxide adsorption on the and graphyne nanosheets for the sensor applications", International Journal of Modern Physics B, 2550108
- 53. Adeleh Vatankhahan, TayebehMovlarooy, "The effect of the width of ribbons and shape of the edges on the electronic and magnetic properties of C6N6 nanoribbons", International Journal of Quantum Chemistry, under revision, 2024.

International conferences

- 1. M. Milko, T. Movlarooy and C. Ambrosch-Draxl, "Light emitting peapods: A first principles study ",USA , 2009 APS March Meeting.
- 2. S. M. Hossein, T. Movlarooy and A. Kompany, "First principles study of electronic properties of PbTiO3 in paraelectric and ferroelectric phases", Modeling, Simulation and Design of Dielectrics, Homerton College, Cambridge, 6-8 April, 2005.
- 3. S. M. Hosseini, T. Movlarooy and A. Kompany, "First principles study of electronic properties of PbTiO3", 13th Multi-disciplinary Iranian Researchers Conference in Europe, Leeds, UK, 2nd July, 2005.
- 4. T.Movlarooy, C. Ambrosch-Draxl and M. Milko, "Oligothiophenes encapsulated in zigzag carbon nanotubes: electronic and optical properties from first principles", workshop on Trends in nanoscience: theory, experiment, technology, Sibiu, Romania, 23-30 Aug, 2009.

- 5. T. Movlarooy, S. M. Hosseini, A. Kompany and N. Shahtahmasebi, "Ab initio study of optical absorption and electron energy loss spectra of SWCNTs", workshop on Trends in nanoscience: theory, experiment, technology, Sibiu, Romania, 23-30 Aug, 2009.
- 6. T. Movlarooy, S. M. Hosseini1, A. Kompany and N. Shahtahmasebi, "Ab initio calculations of electronic structure and optical spectra of (13-0) carbon nanotube", international conference on nano science & technology (ICONSAT 2010), IIT Bombay, Mumbai, India, 17-20 Feb, 2010.
- 7. T. Movlarooy, "DFT study of electronic structure and optical properties of peapod systems", 9th SESAME Users' Meeting, Amman, Jordan, 12 16 November 2011.
- 8. T. Movlarooy, "Ab initio study of electronic structure and optical properties of double-walled carbon and boron-nitride nanotubes", 10th SESAME Users' Meeting, Amman, Jordan, 7 9 November 2012.
- 9. T. Movlarooy, "Large Scale Simulations For Boron Nitride Nanotubes", 10th SESAME Users' Meeting, Amman, Jordan, 7 9 November 2012
- 10. R. Fathi, T. Movlarooy,"Transition metals doped (5,5) GaAs nanotube as a DMS", 3rd International Congress on Nanoscience & Nanotechnology (ICNT2015), Turkey, 2010-06-09
- 11. M. Shabani, T. Movlarooy"Transition metal doped (3 3) armchair GaN nanotube as a DMS", The 5th International Conference on Nanostructures (ICNS5), KISH ISLAND, 2010-06-09
- 12. A. Vatankhahan, T. Movlarooy, Aran Garcia-Lekue "Tuning the electronic and magnetic properties of β12-borophene", Trends in Nanotechnology)TNT 2019, Spain, S a n S e b a s t i a n, 2021-09-06
- 13. R. Fathi, T. Movlarooy, "Transition metal doped (9,0) GaAs nanotube; a diluted magnetic semiconductor", 5th International Congress on Nanoscience & Nanotechnology (ICNN2014), 2010-06-09, Tehran.
- 14. R. Fathi, T. Movlarooy, "Ab initio Study of the Electronic Structure of GaAs Nanotubes", 5th International Congress on Nanoscience & Nanotechnology (ICNN2014), 2010-06-09, Tehran.
- 15. T. Movlarooy, "FIRST PRINCIPLES CALCULATIONS OF DIELECTRIC FUNCTION OF SWCNTS", 3rd International congress on nanoscience and nanotechnology (ICNN 2010), shiraz, 9-11 November 2010.
- 16. T. Movlarooy, "Density functional theory study of a nanohybrid system", 4th Int'l Conf. on Nanostructures (ICNS4), 12-14 Mar 2012, Kish Island, Iran.
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26.to be continue

Considering that the number of articles presented at national conferences is very high, the above cases are examples.