



**Name** : Dr. A. Amudhavalli  
**Designation** : Assistant professor  
**Department** : Physics  
**Date of Birth** : 08.07.1992  
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### Academic Qualification

S. No.	Degree	University / Instituion	Year of Completion
1.	B.Sc.	Fatima College, Madurai	2012
2.	M.Sc.	N.M.S.S.V.N. College, Madurai	2014
3.	M.Phil.	N.M.S.S.V.N. College, Madurai	2015
4.	Ph.D	N.M.S.S.V.N. College, Madurai	2020

**Total Experience : 7 Months**

## **FELLOWSHIPS AND AWARDS**

- Senior Research Fellowship from Council of Scientific and Industrial Research, India.

**Area of Specialization** : Condensed Matter Physics, Computational Physics

### **List of Seminars/ Workshops (Attended / Presented)**

1. National Level Seminar on “Applications of Spectroscopy in Materials Characterization” organized by Department of Physics, Fatima College, Madurai, Tamilnadu held on 22<sup>nd</sup> and 23<sup>rd</sup> August 2012.
2. National Level Seminar on “Recent Trends in Novel Materials” organized by Department of Physics, N.M.S.S.Vellaichamy Nadar College, Madurai, Tamilnadu held on 28<sup>th</sup> February 2013.
3. National Level Seminar on “X-RAY Crystallography” organized by Department of Physics, N.M.S.S.Vellaichamy Nadar College, Madurai, Tamilnadu held on 14<sup>th</sup> February 2014.
4. One day workshop on “Quantum Entanglement” organized by School of Physics, Madurai Kamaraj University, Madurai held on August 25, 2014.
5. Presented a paper entitled “*Structural stability, electronic structure and mechanical properties of alkali gallium hydrides  $AGaH_4$  ( $A = Li, Na$ )*” in the International Conference on Condensed Matter and Applied Physics (ICC 2015) held at Department of Physics, Govt. Engineering College, Bikaner, Rajasthan on October 30 & 31, 2015.
6. Presented a paper entitled “*Structural phase transition, electronic structure and optical properties of half Heusler alloys  $LiBeZ$  ( $Z = As, Sb$ )*” in the 60<sup>th</sup> DAE Solid State Physics Symposium (DAE SSPPS 2015) held at Amity University, Noida, Uttar Pradesh during December 21-25, 2015.
7. National Level Workshop on “Computational Physics using Gaussian” organized by PG and Research Department of Physics N.M.S.S.V.N College, Tamilnadu on February 13, 2015.
8. National Level Workshop on “Current Advances in Nano and Green Chemistry” organized by PG and Research Department of Chemistry, N.M.S.S.V.N College, Tamilnadu on February 18, 2015.
9. National level Seminar on “Nanoscience and Nanotechnology” Organized by Department of Physics, N.M.S.S.Vellaichamy Nadar College, Madurai, Tamilnadu on 19<sup>th</sup> February 2016.

10. One day training on “Faculty Development Programme” organized by N.M.S.S.V.N College, Tamilnadu, on April 1, 2016.
11. Presented a paper entitled “*First Principles Study of Structural Stability and Electronic Structure of 4d Transition Metal Carbides  $TMC_2$  ( $TM= Ru, Rh, Pd$ )*” in the National Conference on Current Advances in Physics (NCCAP- 2017) held at St. John’s College Palayamkottai, Tamilnadu on February 3 & 4, 2017.
12. Workshop on “Quantum Mechanics as a Tool for Materials Investigation” organized by Department of Theoretical Physics, University of Madras, Chennai, Tamilnadu on March 17 & 18, 2017.
13. Presented a paper entitled “*First Principles Study of Co based half metallic Half Heusler Compounds  $CoYBi$  ( $Y = Mn, Cr$ )*” in the International Conference on Energy, Environment and Advanced Materials for a Sustainable Future (ICEEAMSF-2017) held at Kongu Engineering College, Perundurai, Erode on May 23 & 24, 2017.
14. Presented a paper entitled “*Investigation of Structural, Electronic, Mechanical and Optical Properties of Half Heusler Alloys  $LiZnZ$  ( $Z = As, Sb$ )*” in the International Conference on Energy, Environment and Advanced Materials for a Sustainable Future (ICEEAMSF-2017) held at Kongu Engineering College, Perundurai, Erode on May 23 & 24, 2017.
15. Presented a paper entitled “*Structural, Electronic and Magnetic Properties of  $CoMnSb$  and  $NiMnSb$  half Heusler Alloys*” in the National Conference on Advanced Materials and its Applications (NCAMA-2K17) held at The Standard Fireworks Rajaratnam College for Women, Sivakasi on July 6 & 7, 2017.
16. Presented a paper entitled “*Structural, electronic and magnetic properties of  $Fe_2YAl$  ( $Y= Ti, V, Cr$ ) full Heusler alloys*” in the International conference on “Advanced Functional Materials for Energy, Environment and Biomedical Applications” (AFMEEB-2017) held at Madurai Kamaraj University, Madurai on December 11 & 12, 2017.
17. National level Seminar on “Spectroscopic Approaches for Biological and Physical Systems” organized by Department of Physics, N.M.S.S.Vellaichamy Nadar College, Madurai, Tamilnadu on 2<sup>nd</sup> February 2018.
18. Workshop on “Modelling and Simulation in Materials Science and Engineering Workshop” organized by Computational Material Science group, Department of Physics, Sathyabama Institute of Science and Technology, Sathyabama University, Chennai on 18<sup>th</sup> -22<sup>nd</sup> June 2018.
19. Presented a paper entitled “*Electronic and magnetic properties of  $Fe_{2-x}Co_xTiSn$  ( $x= 0, 0.5, 1, 1.5, 2$ ) full Heusler alloys,*” in the International conference on “Nanoscience

and Nanotechnology” (ICONN 2019) held at SRM Institute of Science and Technology, Chennai on January 28-30, 2019.

20. National level Seminar on “Trends in Theoretical Physics” Organized by Department of Physics, N.M.S.S.Vellaichamy Nadar College, Madurai, Tamilnadu on 22<sup>nd</sup> February 2019.
21. National level Conference on “Design and Applications of Emerging Materials” organized by Department of Physics, N.M.S.S.Vellaichamy Nadar College, Madurai, Tamilnadu on 19<sup>th</sup> February 2020.
22. Presented a Paper entitled “*Structural, electronic and magnetic properties of CoCrSb and NiCrSb half Heusler alloys*”, in the National Conference on Functional Materials and its Applicational Aspects (NCFMAA - 2020), held at Saveetha School of Engineering, Saveetha University, Thandalam, Chennai on March 5 & 6, 2020.
23. International Webinar on “Thin Film Technologies in our Daily Life”, organized by Department of Physics, N.M.S.S.Vellaichamy Nadar College, Madurai, Tamilnadu on 30<sup>th</sup> May 2020.
24. Interactive Webinar on “Online Lectures in Solid States Physics (Series- 1: Electrons in Solids)”, organized by Department of Theoretical Physics, University of Madras, Chennai, Tamilnadu on June 1<sup>st</sup> -3<sup>rd</sup>, 2020.

### **List of Publications**

1. Structural stability, electronic structure and mechanical properties of alkali gallium hydrides  $AGaH_4$  ( $A = Li, Na$ ), M. Santhosh, R. Rajeswarapalanichamy, M. Manikandan, A. Murugan, **A. Amudhavalli** and K. Iyakutti, AIP Conf. Proc. 1728 (2016) 020309.
2. Structural phase transition, electronic structure and optical properties of half Heusler alloys  $LiBeZ$  ( $Z = As, Sb$ ), **A. Amudhavalli** and R. Rajeswarapalanichamy, AIP Conf. Proc. 1731 (2016) 030017.
3. First Principles Study of Structural Stability and Electronic Structure of 4d Transition Metal Carbides  $TMC_2$  ( $TM = Ru, Rh, Pd$ ), M. Manikandan, M. Santhosh, **A. Amudhavalli**, R. Rajeswarapalanichamy and K. Iyakutti, IOSR Journal of Applied Physics (IOSR-JAP), e-ISSN: 2278-4861, PP 38-41 (2017).
4. Structural, Electronic and Mechanical Properties of CoN and NiN: An Ab Initio Study, **A. Amudhavalli**, M. Manikandan, A. Jemmy Cinthia, R. Rajeswarapalanichamy and K. Iyakutti, Zeitschrift fur Naturforschung A, A Journal of Physical Sciences, 72 (2017) 321.

5. First principles study of structural and magnetic properties of transition metal nitrides TMN (TM = Cr, Mn), R. Rajeswarapalanichamy, **A. Amudhavalli**, M. Manikandan, M. Kavitha and K. Iyakutti, Phase Transitions 90 (2017) 894.
6. Structural, electronic, mechanical and magnetic properties of Mn based ferromagnetic half Heusler alloys: A first principles study, **A. Amudhavalli**, R. Rajeswarapalanichamy, K. Iyakutti, Journal of Alloys and Compounds 708 (2017) 1216.
7. First principles study on Fe based ferromagnetic quaternary Heusler alloys, **A. Amudhavalli**, R. Rajeswarapalanichamy, K. Iyakutti, Journal of Magnetism and Magnetic Materials 441 (2017) 21.
8. First principles study of structural and optoelectronic properties of Li based half Heusler alloys, **A. Amudhavalli**, R. Rajeswarapalanichamy, K. Iyakutti, A.K. Kushwaha, Computational Condensed Matter 14 (2018) 55.
9. Half metallic ferromagnetism in Ni based half Heusler alloys, **A. Amudhavalli**, R. Rajeswarapalanichamy, K. Iyakutti, Computational Materials Science, 148 (2018) 87.
10. Electronic and Optical Properties of CsSnI<sub>3-y</sub>Cl<sub>y</sub> (y = 0, 1, 2, 3) Perovskites: a DFT Study, R. Padmavathy, **A. Amudhavalli**, M. Manikandan, R. Rajeswarapalanichamy, K. Iyakutti, and A.K. Kushwaha, Journal of Electronic Materials 48 (2018) 1243.
11. Electronic structure, mechanical and optical properties of ternary semiconductors Si<sub>1-x</sub>Ge<sub>x</sub>C (X = 0, 0.25, 0.50, 0.75, 1), M. Manikandan, **A. Amudhavalli**, R. Rajeswarapalanichamy and K. Iyakutti, Philosophical Magazine 99 (2019) 905.
12. Electronic structure and optical properties of CsSnI<sub>3-y</sub>Br<sub>y</sub> (y = 0, 1, 2, 3) perovskites, R. Padmavathy, **A. Amudhavalli**, R. Rajeswarapalanichamy and K. Iyakutti, Int. J. Mod Phys. B, 33 (2019) 1950003.
13. Electronic and optical properties of cubic Perovskites CsPbCl<sub>3-y</sub>I<sub>y</sub> (y = 0, 1, 2, 3), R. Padmavathy, **A. Amudhavalli**, R. Rajeswarapalanichamy and K. Iyakutti, Zeitschrift fur Naturforschung A, A Journal of Physical Sciences, 74 (2019) 905.
14. Electronic and Magnetic properties of Fe<sub>2-x</sub>Co<sub>x</sub>TiGe (x= 0, 0.5, 1, 1.5, 2) full Heusler alloys, **A. Amudhavalli**, M. Manikandan, R. Rajeswarapalanichamy and K. Iyakutti, Chinese Journal of Physics, 59 (2019) 166.
15. Electronic structure and magnetic properties of XMgC (X=Li, Na, K, Rb), M. Manikandan, **A. Amudhavalli**, R. Rajeswarapalanichamy and K. Iyakutti, Solid State Communications, 291 (2019) 36.

16. First principles study of structural, electronic and mechanical properties of metal carbides  $M_2C$  and  $MC_2$  ( $M = Os, Ir, Pt$ ), M. Manikandan, **A. Amudhavalli**, R.Rajeswarapalanichamy and K. Iyakutti, Solid State Communications, 291 (2019) 43.
17. Electronic and Magnetic Properties of  $Fe_{2-x}Co_xTiSi$  ( $x= 0, 0.5, 1, 1.5, 2$ ) Heusler Alloys, **A. Amudhavalli**, R.Rajeswarapalanichamy and K. Iyakutti, Journal of Electronic Materials, 48 (2019) 6753.
18. Investigation of half- metallic and magnetic phase transition in  $Co_2TiZ$  ( $Z= Al, Ga, In$ ) Heusler alloys, **A. Amudhavalli**, R.Rajeswarapalanichamy and K. Iyakutti, Phase Transitions, 92 (2019) 875.
19. First-principles study of structural and optoelectronic properties of  $CsSnI_{3-y}F_y$  ( $y = 0, 1, 2, 3$ ) perovskites, **A. Amudhavalli**, R.Padmavathy, R.Rajeswarapalanichamy and K. Iyakutti, Indian Journal of Physics(2020), DOI: 10.1007/s12648-019-01598-1
20. Band gap engineering in halide cubic perovskites  $CsPbBr_{3-y}I_y$  ( $y = 0, 1, 2, 3$ ) – A DFT study, R.Rajeswarapalanichamy, **A. Amudhavalli**, R.Padmavathy, and K. Iyakutti, Materials Science and Engineering: B, 258 (2020) 114560.
21. Investigation of phase transition in electronic structure and magnetic properties of  $Fe_{2-x}Co_xTiSn$  Heusler alloys, **A. Amudhavalli** and R.Rajeswarapalanichamy, Phase Transitions, (2020) DOI: 10.1080/01411594.2020.1768256.
22. Structural, electronic and mechanical properties of  $AgIn_{1-x}Ga_xS_2$  ( $X= 0, 0.25, 0.5, 0.75, 1$ ) Chalcogenides, R. Padmavathy, **A. Amudhavalli**, R. Rajeswarapalanichamy and K. Iyakutti, Indian Journal of Physics, DOI: 10.1007/s12648-020-01841-0.
23. Electronic structure, elastic, optical and thermal properties of chalcopyrite  $CuBY_2$  ( $B = In, Ga, In_{0.5}Ga_{0.5}; Y = S, Se, Te$ ) solar cell compounds, **A. Amudhavalli**, R.Rajeswarapalanichamy, R.Padmavathy, M. Manikandan, M. Santhosh, K. Iyakutti, Materials Today Communications, 26 (2021) 101790
24. Electronic Structure and Optical Properties of  $CsPbF_{3-y}I_y$  ( $y=0,1,2$ ) Cubic Perovskites, **A. Amudhavalli**, R.Rajeswarapalanichamy, R.Padmavathy, K. Iyakutti, Acta Physica Polonica Series a 139(6) (2021) 692-697
25. Electronic structure, magnetic, optical and transport properties of half-Heusler alloys  $RhFeZ$  ( $Z = P, As, Sb, Sn, Si, Ge, Ga, In, Al$ ) – a DFT study, R. Meenakshi, R. Aram Senthil Srinivasan, **A. Amudhavalli**, R.Rajeswarapalanichamy, K. Iyakutti, Phase Transitions 94(2021) 1-21.

26. Electronic, Magnetic, and Mechanical Properties of  $YX'CrZ$  ( $X' = Fe, Co, Ni$ ;  $Z = Si, Ge, Sn$ ) Quaternary Heusler Alloys, **A. Amudhavalli**, M. Santhosh, P. Dharmaraja, M. Manikandan, R.Rajeswarapalanichamy, Journal of Superconductivity and Novel Magnetism (2021). DOI: 10.1007/s10948-021-05975-y

**Seminars/Conference/Workshops Participated (Last five Years): 13**