# DEPARTMENT OF HUMANITIES AND SCIENCES PHYSICS

Name : Lt. Dr. E.VISWANATHAN

Designation : ASSOCIATE PROFESSOR

DOB : 24-11-1988

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Oualification :



UG	B.E/B.Tech/B.Sc./ B.A./BBA/B.Ed.	Date of Completion	University	% of Marks	Class
	B.Sc Physics	May 2009	Bharathidasan Univeristy	81.2	Distinction
PG	M.E/M.Tech/ M.Sc./ M.A./MBA/M.Ed	Date of Completion	University	% of Marks	Class
	M.Sc Physics	May 2012	Bharathidasan Univeristy	89.7	Distinction
Ph.D	Date of Completion	Field of Specialization	University	NA	NA
	Thesis submitted	Condensed Matter Physics	Sathyabama Institute of Science and Technology		
SLET Marks	NET Marks	Date of Eligibility Sep 2017	-	-	-

Area of Specialization: Computational Condensed Matter Physics

Research Interest : Density Functional theory

Experience in years : Teaching : 6 y 3 m Research: - Industry: - Others:

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Courses Taught in UG / PG Level:

- 1.Engineering Physics
- 2. Physics for Information Scinece
- 3. Physics of Materials

No. of Workshop/Conferences/ FDP attended : Workshop: 3 Conferences: 3

FDP: -

No. of Workshop/Conferences/ FDP Organized : Workshop: 1 Conferences: -

FDP: -

Professional Membership	IEEE membership					
	No. of papers published in National Journals / Conferences : 6					
	No. of papers published in International Journals / Conferences: 21					
	No. of Books published : 1					
Publications	Name of the Book	ISBN No: Year of Publication				
	Thermoelectric properties of BaFe <sub>2</sub> As <sub>2</sub> and Ba <sub>2</sub> FeAs <sub>2</sub> Compounds	978-620-2-31424-4	2018			
	No.Of UG Students Guided:-Nil-					
Research Guidance	No.Of PG Students Guided: -Nil-					
	No.Of Ph.Ds Guided: -Nil-					
Research Funded Projects	-Nil-					
Patents	Filed: -Nil- Granted: -Nil-					
Technology Transfer	-Nil-					
Achievements  Received Course Best Firer Award 2023 (Associate NCC Officer during 12 <sup>th</sup> Aug to 9 <sup>th</sup> Sep, 2023 at NCC-OTA, Kamptee)						
	PhD Supervisor Recognition from Anna University 4170039					
Any Other Information	Completed Pre-Commission course for Associate NCC Officer during 12 <sup>th</sup> Aug to 9 <sup>th</sup> Sep, 2023 at NCC-OTA, Kamptee and commissioned as Lieutenant.					

# **Teaching and Research Experience**

2019-2020	Assistant Professor, Department of Physics, National College, Trichy	
2013-2016	Junior Research Fellow in DST-SERB, India funded Project, Sathyabama University, Chennai	
2013-2019	Lab Assistant - M.Sc Physics Laboratory	
	Sathyabama University, Chennai	
2017-2019	Instrument Handling in DST-FIST Lab (TGA, FTIR), Sathyabama University, Chennai	

## Publications.

- Gayathri Chellasamy, Shiva Kumar Arumugasamy, Satheesh Kuppusamy, Viswanathan Ekambaram, Kandeeban Rajagopalan, Sada Venkateswarlu, Prabhakaran Deivasigamani, Min Jae Choi, Saravanan Govindaraju, Kyusik Yun, <u>MXene–MOF architectural hybrid-supported nickel single-atom catalysts for hydrogen evolution reactions</u>, Journal of Materials Chemistry A, 12, 2, 1115-1127, 2024, <a href="https://doi.org/10.1039/D3TA06045D">https://doi.org/10.1039/D3TA06045D</a>.
- 2. Manjula M, Krishnaveni S, **Viswanathan E**, Muthumari M, Influence of Rb doping in optical and thermoelectric properties of KCl A DFT approach, Materials Today: Proceedings, 50, 7, 2729-2736, 2022, https://doi.org//10.1016/j.matpr.2020.08.271.
- 3. Priyadharshini S., Sundareswari M., **Viswanathan E**, Jayalakshmi D S, Manjula, M., Band engineering of modified rhombohedral Cu<sub>4</sub>Mn<sub>2</sub>Te<sub>4</sub>:ab initio approach, Philosophical Magazine, 102, 13, 1261-1289, 2022, https://doi.org//10.1080/14786435.2021.2023774.
- 4. Manjula M, **Viswanathan E**, Muthumari M, Pradheepa K, Dhivyabharathi R, Shalini L, Kuznetsov Denis, Veluswamy Pandiyarasan, Lifting the Optical and Thermoelectric Properties of Mg<sub>2</sub>Si as a Function of Sn Incorporation—Potential Thermoelectric Materials, ECS Journal of Solid State Science and Technology, 10, 7, 071023, 2021, https://doi.org//10.1149/2162-8777/ac1479.
- 5. Jayalakshmi D S, **Viswanathan E**, Sundareswari M, Hemanand D, Theoretical investigation of thermoelectric property and damage tolerance of LuB<sub>2</sub>C<sub>2</sub> compound, Computational Condensed Matter, 2021, 28, e00566. https://doi.org/10.1016/j.cocom.2021.e00566.
- 6. Muthumari M, Manjula M, Sundareswari M, **Viswanathan E**, Investigation on half-metallic ferromagnetism in Phosphorous doped SmN-Band structure study, Journal of Physics: Conference Series, 1770, 1, 012093, 2021, <a href="https://doi.org/10.1088/1742-6596/1770/1/012093">https://doi.org/10.1088/1742-6596/1770/1/012093</a>.
- 7. Manjula M, Malliga P, **Viswanathan E**, Muthumari M, Ab-initio investigations of electronic, optical, mechanical and thermal properties of Ca<sub>0.875</sub>Ba<sub>0.125</sub>Te, Journal of Physics: Conference Series, 1770, 1, 012094, 2021, <a href="https://doi.org/10.1088/1742-6596/1770/1/012094">https://doi.org/10.1088/1742-6596/1770/1/012094</a>.
- 8. Priyadharshini S, Sundareswari M, **Viswanathan** E, First principles band structure investigation of cubic spinel CuMn<sub>2</sub>Te<sub>4</sub> Compound for thermoelectric applications, Journal of Physics: Conference Series, 2070, 1, 012037, 2021, <a href="https://doi.org/10.1088/1742-6596/2070/1/012037">https://doi.org/10.1088/1742-6596/2070/1/012037</a>.
- 9. Jayalakshmi D S, Sundareswari M, **Viswanathan E** and Leena Josphine, "Lifshitz transition on SrFe<sub>2</sub>As<sub>2</sub> and SrFe<sub>2</sub>Bi<sub>2</sub> compounds under pressure", Proceedings of the Indian National Science Academy, 86, 3, 1279-1286, 2020.
  - https://doi.org/10.16943/ptinsa/2019/49671.
- 10. M.Manjula, S.Krishnaveni, E.Viswanathan, M.Muthumari, "Influence of Rb doping

- in optical and thermoelectric properties of KCl A DFT approach", Materials Today Proceedings, Accepted on 5-10-2020. <a href="https://doi.org/10.1016/j.matpr.2020.08.271">https://doi.org/10.1016/j.matpr.2020.08.271</a>.
- 11. D. S. Jayalakshmi, M. Sundareswari, **E. Viswanathan**, D. Hemanand and Venkat Pranesh, "Computational study on unconventional superconductivity and mechanical properties of novel antiferrromagnetic (Ca,Sr,Ba)Fe<sub>2</sub>Bi<sub>2</sub> compounds", International Journal of Modern Physics B, 33, 28, 1950341, 2019. <a href="https://doi.org/10.1142/S0217979219503417">https://doi.org/10.1142/S0217979219503417</a>.
- 12. **E.Viswanthan**, M.Sundareswari, S.Krishnaveni, M.Manjula, D.S.Jayalakshmi, "Theoretical Investigation on Effect of Boron on Improving the Hardness of Cubic Zincblende-Aluminium Nitride and Its Mechanical, Thermal and Thermoelectric Properties", Journal of Superhard Materials, 41, 5, 321-333, 2019. https://doi.org/10.3103/S1063457619050046.
- 13. D.S.Jayalakshmi, M.Sundareswari, **E.Viswanathan**, "Theoretical Prediction of Possible Coexis-tence of Superconductivity and Antiferromagnetism in Novel SrFeRuBi2, SrRu2Bi2 and Parent SrFe2Bi2 Compounds", Scientific Bulletin series A, 81, 2, 221-232, 2019. https://www.scientificbulletin.upb.ro/rev\_docs\_arhiva/fullcac\_116981.pdf.
- 14. **E.Viswanathan**, M.Sundareswari, D.S.Jayalakshmi, M.Manjula, "Fermi Surface and Hardness Enhancement Study on Ternary Scandium and Vanadium Based Borides by First Principles Investigation", Computational Materials Science, 157, 107-120, 2019.

(https://doi.org/10.1016/j.commatsci.2018.10.040).

- 15. D.S.Jayalakshmi, M.Sundareswari, **E.Viswanathan**, Abhijeet Das, "Theoretical investigation on thermoelectric properties of (Ca,Sr, Ba)Fe2(As,Bi)2 compounds under temperature", AIP Conference Proceedings, 1951, 020002-1 020002-7, 2018. (https://doi.org/10.1063/1.5031710).
- 16. M.Manjula, M.Sundareswari\* and **E.Viswanathan**, "Effect of Zr substitution on the thermal and mechanical properties of Rh3A (A=Nb,Ta) A theoretical study", AIP Conference Proceedings, 1951, 030015-1 030015-7, 2018. (https://doi.org/10.1063/1.5031741).
- 17. M.Manjula, M.Sundareswari and **E.Viswanathan**, "Elastic and Thermodynamic Properties of Zirconium and Hafnium doped Rh3V Intermetallic Compound- Potential Aerospace Material, Bulletin of Materials Science, 41, 19, 2018. (https://doi.org/10.1007/s12034-017-1537-3).
- 18. **E.Viswanathan**, M.Sundareswari, D.S.Jayalakshmi, M.Manjula, S.Krishnaveni, "Structural, electronic, mechanical, thermal and optical properties of B(P,As)1-xNx; (x=0, 0.25, 0.5, 0.75, 1) alloys and hardness of B(P,As) under compression using DFT calculations, Indian Journal of Physics, 91, 9, 999-1011, 2017. (https://doi.org/10.1007/s12648-017-0996-0).
- 19. M.Manjula, M.Sundareswari, **E.Viswanathan**, "Enhancement of ductility in cubic Rh3AxTi1-x(A= V, Nb, Ta)(x= 0, 0.125, 0.25, 0.75, 0.875, 1) aerospace materials First principles DFT study, Materials Chemistry and Physics (Elsevier) 1, 9, 1-9, 2016.

(https://doi.org/10.1016/j.matchemphys.2016.06.037).

- 20. M.Sundareswari, D.S.Jayalakshmi and **E.Viswanthan**, A first principles study on newly proposed (Ca/Sr/Ba)Fe2Bi2 compounds with their parent compounds, Philosophical Magazine, 96, No 5, pp, 511-523, 2016. https://doi.org/10.1080/14786435.2016.1140911).
- 21. R.Sugan Harish, D.S.Jayalakshmi, **E.Viswanathan** and M.Sundareswari, Structural stability, electronic, mechanical and thermo dynamical properties of CaNi2P2 and CaNi2Sb2 compounds by band structure calculations, Modern Physics Letters B, 30, No.12, 1650178, 2016.

# (https://doi.org/10.1142/S0217984916501785).

22. **E.Viswanathan**, M.Sundareswari, Study on structural, electronic and elastic properties of boron arsenide doped with nitrogen using density functional theory, Journal of Chemical and Pharmaceutical Sciences, Spl Iss. 11, 11-14, 2015.

(https://www.jchps.com/specialissues/Special issue 11/jchps 4 E.Viswanathan 11-14.pdf).

23. **E.Viswanathan**, M.Sundareswari, D.S.Jayalakshmi and M.Manjula, Theoretical investigation on structural and electronic properties of PdO2, AIP Conference Proceedings, 1665, 090047, 2015.

(https://doi.org/10.1063/1.4918027).

24. S. Krishnaveni, M. Sundareswari and **E.Viswanathan**, Computational study of structural and electronic property of the predicted compound-Os2TiBi, Journal of Chemical and Pharmaceutical Research, 2015, 7(2):378-380.

(<a href="http://www.jocpr.com/articles/computational-study-of-structural-and-electronic-property-of-thepredicted-compoundos2tibi.pdf">http://www.jocpr.com/articles/computational-study-of-structural-and-electronic-property-of-thepredicted-compoundos2tibi.pdf</a>).

25. M.Manjula, M.Sundareswari, D.S.Jayalakshmi and **E.Viswanathan**, Theoretical investigation on improving the ductility of Rh3V by ternary addition, AIP Conference Proceedings, 1665, 090046, 2015. (https://doi.org/10.1063/1.4918026).

#### **Books**

1. Jayalakshmi, D.S., Sundareswari, M., **Viswanathan, E.,** Das, Abhijeet Das, Thermoelectric properties of BaFe<sub>2</sub>As<sub>2</sub> and Ba<sub>2</sub>FeAs<sub>2</sub> Compounds, Scholar's Press, pp 1-56, 2018, ISBN-978-620-2-31424-4.

## Workshop organized/tutored

- 1. As a co-convener organized a CSIR sponsored summer workshop on "Modelling and Simulation in Materials Science and Engineering" with hands on session (MSME 2018), during 18-22, June 2018, at the Department of Physics, Sathyabama Institute of Science and Technology, Chennai—119.
- 2. Acted as a tutor in the CSIR Sponsored Winter School on Computational Modelling (WISCOM-2020) during 27-29, Feb, 2020 held at PG & Research Department of Physics, Holy Cross College, Trichy.

#### Reviewer

1. Reviewer in a 'International Journal of Computational Materials Science and Engineering.

# **Award**

1. Received best firer award during the Pre-Commission course for Associate NCC Officer during 12<sup>th</sup> Aug to 9<sup>th</sup> Sep, 2023 at NCC-OTA, Kamptee.

# Major Workshop/Internship/School Attended

National Work Shop On "Advanced Techniques Related To Analytical, Molecular, Material Testing And Statistical Tools" (NWAT-2018)

27th -29th March 2018

Andhra University

Participated in "INDO-French Workshop on Pressure Effects on Strongly Correlated Materials IWPESCM17"

9-12, January 2017

Bharathidasan University

Participated in the SERB School on "Density Functional Theory and Beyond: Computational Materials Science and Materials Design"

24th November – 13th December 2014

The M.S. University of Baroda

Summer Internship Programme 16th May – 15th July, 2011. (Summer School & Project) Indian Institute of Astrophysics

"Third Science Conclave-2010 Interaction Programme with 8-14 Dec – 2010 Noble Laureates"

Indian Institute of Information Technology, Allahabad, UP.

# Major Conferences/ Seminar/ Guest Lecture Attended

Advances in Refractory and Reactive Metals and 27-29, January 2016

Alloys(ARRMA 2016) Bhabha Atomic Research Centre.

Preconference Meet with Nobel Laureate Dr. 5-6, December 2013

Walter Kohn (ICRAPID 2014) Sathyabama University.

One day training programme on Effective 24th January, 2017

Teaching" IQAC, Sathyabama University

National Seminar on "Quality Higher Education 28-29, April 2017

2017" IQAC, Sathyabama University.

# **Conference presented**

Using Density Functional Theory)

(Oral) Presented in one day seminar on "Sensors" entitled
"Synthesis and characterization of Nanoporous Pigment for the Identification of Hazardous air pollution"

28th October 2017.

MIT Campus, Anna University

(Oral) Presented in TEQIP-II Sponsored International
 Conference on Recent Advancements in Materials
 (ICRAM-2015) entitled (Study on Structural, Electronic and Elastic Properties of Boron Arsenide Doped with Nitrogen

Trichy Campus, Anna University

(Poster) 59th DAE Solid State Physics Symposium – Presented a paper "Theoretical Investigation on structural and electronic Properties of PdO2"

16-20, December 2014VIT University, Vellore.

## **Academic Workload**

2. Theory Papers Handled for I B.E/B.Tech Students

Engineering Physics, Physics for Information Science, Physics of Materials and Physics of Electronic Devices

3. Laboratory Handling

Major Laboratory – I yr B.E/B.Tech Students

# **Technical Skills**

- 4. Working experience with software packages like Wien2k, VASP, Origin, VESTA, BoltzTraP, Elastic 1.0, ELATE, GIBBS and Xcrysden.
- 5. Hands on experience with operating system like Windows and Linus Cent OS, Ubuntu, Open Suse.

# **Research Interest**

With the trustworthy computational codes and effective ab initio density functional theory, computational materials science plays a major role in predicting material's properties. In many areas, the computations reached an appreciable level of accuracy often analogous to the experimental data. These theoretical models play a key role in trends of correlating properties of materials and provide clue for the synthesis of novel class of materials.

I am working on superhard materials especially covalent bonded crystalline materials such as borides, nitrides and carbides. Hardness is very resourceful and a quick strength probe among the mechanical properties. Though the hardest superhard materials like diamond and cBN find excellent applications, its disadvantages lead to necessity of development of alternate superhard materials.

I am using Wien2k and VASP package to study the band/electronic structure calculation and also other properties such as structural changes under pressure, Fermi surface for metals, mechanical properties like stiffness coefficients, elastic moduli namely Young's, bulk and shear modulus and Poisson's ratio, Pugh's ratio, Cauchy'c criteria, Kleinman parameter, Cauchy and Born ratio, anisotropy, hardness, ductility/brittleness, thermal properties like Debye temperature, elastic wave velocity, melting temperature, transport properties like Seebeck coefficient, electrical conductivity/resistivity, electronic thermal conductivity, optical properties like real and imaginary part of dielectric constant, refractive index, extinction coefficient, reflectivity, etc.