

Curriculum vitae

Prof. Dr. P. Ravindran
(June, 2023)



PERSONAL DATA

Present Designation	Professor and Head at Department of Physics, Head, Simulation Center for Atomic and Nanoscale MATerials (SCANMAT) Central University of Tamil Nadu, India Within top 1% scientists in the world in Applied Physics. (Stanford University Study) Rank 13 in National level (SCOPUS study).
Address	Department of Physics School of Basic and Applied Sciences, Central University of Tamil Nadu, Neelakudi, Kandalanchery, Thiruvarur 610 005. Email: raviphy@cutn.ac.in ;or ponravi67@gmail.com Phone Office : +91 9489054267 Mobile: +91 8300178007 URL: https://folk.universitetetioslo.no/ravi/cutn/
Date of Birth	04-05-1967
Sex and Marital status	Male, Married
Nationality	Indian
Languages known	Tamil (Mother Tongue) English Norwegian – Good; Swedish - Fair

ACADEMIC QUALIFICATIONS

Ph. D Solid State Physics 1996	Anna University, Madras, INDIA (Highly Commended) Title of the thesis: <i>Electronic structure, Phase stability and equation of state studies on structural and superconducting intermetallics.</i>
M. Sc Physics (specialization Materials Science) 1989	Anna University, Madras, INDIA (First Class) M.Sc dissertation entitled <i>XRD and SAXS investigation on $YBa_2Cu_3O_{7-x}$</i>
B. Sc Physics 1987	Madurai Kamaraj University, INDIA (First Class)

AWARDS

- ❖ 2020, 2021 & 2022 Listed among top 2% of Scientist in the world in Applied Physics by a study from Stanford University, USA
- ❖ 2022 listed as 13th rank in Indian level scientist in Applied Physics by SCOPUS ranking.
- ❖ 2019 Member, American Chemical Society
- ❖ 2014 Elected as Fellow of the Academy of Sciences, Chennai, India.

- ❖ **2013** Adjunct Professor, Center for Materials Science and Nanotechnology, Univ. of Oslo, Norway
- ❖ **2011 to 2016** Steering Committee member of European Science Foundation- Ψ_k etwork- Representing Norway.
- ❖ **1998** Postdoctoral Fellowship from Research Council of Norway (RCN), Norway.
- ❖ **1996** Forskarassistentjaenst (Guest Researcher) from Swedish Natural Science Research Council (NFR), Sweden.
- ❖ **1996** Research Associate Fellowship award of Council of Scientific and Industrial Research (CSIR), India.
- ❖ **1994** Senior Research Fellowship award of CSIR, India.
- ❖ **1992** Senior Research Fellowship (SRF) award of Department of Atomic Energy (DAE), India
- ❖ **1990** Junior Research Fellowship award of Department of Atomic Energy (DAE), India
- ❖ **1989** Project Associate Fellowship at IIT-Madras, by Indian Space Research Organization (ISRO), India.
- ❖ **1989** First rank in M.Sc. Thesis presentation, Anna University, Chennai, India.

EMPLOYMENT AND RESEARCH EXPERIENCE

Name of Institution	Period		Academic Position and Funding Agency
	From	To	
Project Cell, Central University of Tamil Nadu, India	15.06.2023	Till date	Head
Central University of Tamil Nadu, India	24.0.2023	Till date	Dean of Research
Department of Physics, School of Basic and Applied Sciences, Central University of Tamil Nadu, India	24.02.2023	Till date	Head
Project Cell, Central University of Tamil Nadu, India	22.08.2019	23.04.2021	Head
Simulation Center for Atomic and Nanoscale Materials (SCANMAT), Central University of Tamil Nadu, India	24.10.2016	Till date	Head
Department of Materials Science, School of Technology, Central University of Tamil Nadu, India	30.03.2016	11.4.2018	Professor & Head
Central University of Tamil Nadu, India	14-07-2014	31.7.2015	Registrar (Acting)
Department of Physics, School of Basic and Applied Sciences, Central University of Tamil Nadu, India	19-03-2012	15-7-2014	Head
Department of Physics, School of Basic and Applied Sciences, Central University of Tamil Nadu, India	19-03-2012	Till date	Professor
Center for Materials Science and Nanotechnology University of Oslo, NORWAY.	01-04-2013	31.03.2018	Adjunct Professor University of Oslo
Center for Materials Science and Nanotechnology University of Oslo, NORWAY.	01-10-2005	18-03-2012	Forsker(Research Professor) University of Oslo
Institute for Energy Technology (IFE), University of Oslo, NORWAY.	01.10.2004	30.09.2005	Research Scientist University of Oslo
Department of Chemistry, University of Oslo, NORWAY.	15-11-2002	30-09-2004	Associate Professor University of Oslo
Department of Chemistry, University of Oslo, NORWAY.	01-12-1998	14-11-2002	Postdoctoral Fellow University of Oslo (NFR-NORWAY)

Condensed Matter Theory Group, Department of Physics, Uppsala University, SWEDEN.	21-05-1996	30-11-1998	Postdoctoral Fellow NFR-SWEDEN
Low Temperature and Superconductor Lab., Materials Science Division, Indira Gandhi Centre for Atomic Research, Kalpakkam, INDIA.	01-01-1996	15-05-1996	Research Associate CSIR-INDIA
Department of Physics, Anna University, Madras, INDIA.	01-02-1994	31-12-1995	Senior Research Fellow , CSIR-INDIA
Department of Physics, Anna University, Madras INDIA.	03-03-1992	31-01-1994	Senior Research Fellow , DAE-INDIA
Department of Physics, Anna University, Madras, INDIA.	02-03-1990	02-03-1992	Junior Research Fellow , DAE-INDIA
Department of Chemical Engg., Indian Institute of Technology, Madras, INDIA.	06-09-1989	30-11-1989	Project Associate ISRO-INDIA

RESEARCH AREAS OF INTEREST

Electronic structure studies on solids using state-of-the-art density functional methods.

❖ General Interest

- Nanophase materials
- MOFs and other nano/micro/meso-porous materials
- Hydrogen Storage & Battery Materials
- Solar Energy Materials including Transparent conducting oxides
- Defects in semiconductors
- Linear, nonlinear optical properties and other Excited State properties
- Magneto-optical and Magneto-caloric materials.
- Magnetic properties, Magnetic anisotropy, Spin, Charge and Orbital ordering
- Multi-ferroic and other multifunctional materials
- Structural Phase Stability and High Pressure studies
- Theory of Alloy Formation
- Thermoelectrics
- Mechanical properties of structural/aerospace engineering materials
- Superconductivity and phonons
- Catalytic Materials
- Materials informatics

❖ Special interest

Stability and functional properties of nanophase materials — Phase stability and Phase diagram studies — Site occupancy studies — mechanical properties of structural intermetallics — Pressure induced structural transition — Elastic properties and calculation of single crystal elastic constants — Zone boundary phonons calculation — Pressure induced superconductivity — Role of interstitials in magnetic, superconducting and mechanical properties of intermetallics — High- T_c superconductors — Insulator-to-metal transition — Spin-state and valence transition — Optical properties of ferro-electrics, nonlinear optical crystals — Magneto-optics — Kerr and Faraday spectra — Raman, XANES, XPS, UPS, XES and BIS spectra — Ferro-, Ferri-, Antiferro-, and noncollinear-magnetism — Magneto crystalline anisotropy — Mössbauer data (HFF, EFG, QS, IS) —Ferroelectric properties of multiferroics — CMR and GMR materials — Spin-, Charge-, and Orbital-ordering — Hydrogen storage materials — Li ion battery materials, thermoelectrics, Solar energy materials — Transparent conducting oxides — Low dimensional systems such as surfaces, interfaces and

multilayers – Materials of geophysical interest – Multiferroics – Magnetocaloric materials – Defects in semiconductors – Transport properties of thermoelectric materials – Optical properties using GW, BSE and TDDFT methods, photo-catalysts - vdW DF method – machine learning.

More details on some of my research activities can be found in <http://folk.uio.no/ravi/activities.htm>

SCIENTIFIC COMPETENCE

I have independently built a materials modeling activity from the scratch in an experimental Solid State Chemistry group at University of Oslo - Purchasing, installing and maintaining computational codes at supercomputers – Identifying interesting problems for co-workers and devising methodologies to solve them – Initiating collaborations – Attracting external funding.

Program Development

Part of my research activity is to develop computer programs. I have developed computer programs for calculating

- ❖ Magneto-optical properties – Kerr, Faraday spectra and figure-of-merit
- ❖ Linear optical properties – Reflectivity, absorption co-efficient with appropriate broadening
- ❖ Single crystal elastic constants for low symmetric crystals (First person to apply density functional theory for calculating elastic properties of orthorhombic and monoclinic crystals)
- ❖ 3D visualization of mechanical properties
- ❖ Ferroelectric properties (Born effective charges, site projected and total polarization).
- ❖ IR and Raman active phonons
- ❖ XPS, UPS and BIS spectra
- ❖ Fermi surface properties – implemented in Wien 95 code
- ❖ Methodology to build and analyze nanophase materials
- ❖ Fitting program to calculate Gibbs free energy, bulk modulus, and its pressure derivative from different equations of states
- ❖ Electron-phonon coupling constant using Rigid muffin-tin approximation
- ❖ Superconducting transition temperature using McMillan's formula
- ❖ Tools for 3D visualization of charge and orbital ordering
- ❖ Developed plotting packages, routines for data analysis as well as physical properties studies
- ❖ Introduced new ICSD-based methodology for structure prediction.

Computational Knowledge

I have installed and maintaining the following advanced density functional programmes in local computers as well as at the Norwegian supercomputer facilities:

- Tight Binding Linear Muffin-tin Orbital (TBLMTO) code – from MPI, Stuttgart, Germany
- Full-Potential Linear Augmented Plane Wave code (WIEN2k)- Technical Univ. Wien, Austria
- Full-Potential Linear Muffin-tin Orbital code (FPLMTO) – Los Alamos National Lab., USA
- Projector Augmented Plane Wave and Pseudopotential Code (VASP5) - Univ. of Wien, Austria
- Linear combination of atomic orbital and Pseudopotential Code (CRYSTAL06) – Univ. of Torino, Italy.
- CASTEP, ONETEP, DMol3.
- PHONON
- ABINIT

Very good experience in installing and maintaining these codes in advanced computers such as SUN, DEC, IBM-SP4, HP-UX-9000, SGI-Origin3800L, CRAY T3E, J90 and Linux clusters with various environments etc. WIEN2k, FPLMTO, CRYSTAL06, ABINIT, DMOL3, CASTEP, and VASP are running in parallel mode in NOTUR supercomputer facilities.

Establishment of Laboratories:

I am the key person to establish Central Instrumentation facility, High performance computing facility, Browsing center for students, Mechanics Lab, Atomic and Molecular Physics Lab, Condensed Matter Physics Lab, Electricity and Magnetism lab, Optics Lab, Heat and Thermodynamics lab, and Computational Physics Lab in Central University of Tamil Nadu (CUTN). I have actively involved in bringing internet and Wi-Fi facilities in CUTN. I have spent substantial amount of time to design interiors of buildings for the School of Basic and Applied Sciences.

Research Grants and Proposals:

S.No	Project Title and Fund Received	Duration		Completed /On-going	Funding Agency
		From	To		
1.	Electronic structure and Phase stability study on superconductors	01.01.1996	31.05.1997	Completed	CSIR-India
2.	Density functional studies on excited state properties of intermetallics	30.06.1997	30.11.1998	Completed	Research Council of Sweden (NFR)
3.	Theoretical Investigation on Perovskite Oxides	01.12.1998	15.11.2000	Completed	Research Council of Norway
4.	First-principles Investigations of Ferroelectric and Superconducting Materials	01.01.2000	01.01.2002	Completed	Research Council of Austria (FWF)
5.	Films, interfaces and nanomaterials	16.11.2000	16.11.2002	Completed	Research Council of Norway
6.	Theoretical exploration on electronic structure, magnetic, and other interesting properties of complex oxides	2002	2006	Completed	Research Council of Norway
7.	Optical and magneto-optical properties of inorganic solids from density functional calculation	2003	2005	Completed	Research Council of Norway
8.	Electronic Structure and structural properties of electro-ceramics	2003	2006	Completed	Research Council of Norway
9.	Oxides for Future information and communication technology;	01.10.2003	30.06.2007	Completed	Research Council of Norway
8.	Theoretical exploration on electronic structure, magnetic, and other interesting properties of complex oxides	2002	2006	Completed	Research Council of Norway
9.	Optical and magneto-optical properties of inorganic solids from density functional calculation	2003	2005	Completed	Research Council of Norway
10.	Electronic Structure and structural properties of electro-ceramics	2003	2006	Completed	Research Council of Norway
11.	Oxides for Future information and communication technology; NFR project no.: 185309/S30	2003	2007	Completed	Research Council of Norway

12.	Theoretical Investigation of Hydrogen Storage Materials	2003	2011	Completed	Research Council of Norway
13.	Design of multiferroic magneto-electric materials	2007	2009	Completed	Research Council of Norway
14.	Design and understanding of solar Materials at the Nanoscale	2007	2011	Completed	Research Council of Norway
15.	Nordic Center of Excellence on Hydrogen Storage Materials	2007	2011	Completed	Research Council of Norway
16.	Novel Nanocomposites for Hydrogen Storage Application	2007	2011	Completed	European Union 7 Frame work program
17.	Conducting Oxides and Nanostructures for Energy technology ISP - CONE	2007	2012	Completed	Research Council of Norway
18.	Theoretical exploration of magnetic oxide thin films	2008	2010	Completed	Research Council of Norway
19.	Exploration of Next-Generation Solar-Energy Materials	2009	2011	Completed	Research Council of Norway
20.	Magnetocaloric materials for environmental-friendly efficient refrigeration	2009	2011	Completed	Research Council of Norway
21.	Design of nanostructured multiferroic magnetoelectric materials	2009	2011	Completed	Research Council of Norway
22.	Computational Materials Science: Atomic and Nanoscale Modeling of Advanced Materials	2010	2011	Completed	Research Council of Norway
23.	Optical properties of transparent conducting oxides and their interfaces	2010	2011	Completed	European Union via European Theoretical Spectroscopy Facility
24.	Nanophase Materials for Hydrogen-storage applications – <i>Indo-Norwegian (INDNOR) Program</i>	2010	2011	Completed	Research Council of Norway & Dept. of Science & Technology (DST), India
25.	Development of High-Efficiency Photovoltaic Oxides	2010	2012	Completed	Research Council of Norway
26.	Design of nanostructured multiferroic magnetoelectric materials	2010	2012	Completed	Research Council of Norway

27.	Design of Efficient Solar Energy Materials from Theory	2010	2012	Completed	Research Council of Norway
28.	<i>Indo-Norwegian Collaboration on Solar Energy</i>	2011	2012	Completed	INDNOR program of Research Council of Norway
29.	Nano-Materials for Improved Lithium Batteries	2011	2014	Completed	Research Council of Norway
30.	Research Networking Program on Advanced Concepts in ab-initio Simulations of Materials (Psi-k)	2011	2017	Completed	European Science Foundation,
31.	Development of High Energy Lithium Batteries	2012	2013	Completed	Research Council of Norway
32.	Create a Department of Materials Science and Nanotechnology at CUTN to launch MTech and IMSc program	2012	2017	Completed	UGC 12 th FYP
33.	Create a Department of Energy and Environmental Sciences at CUTN to launch MTech and IMSc program	2012	2017	On going	UGC 12 th FYP
34.	Create an interdisciplinary center titles <i>Simulation Center for Atomic and Nanoscale MATerials (SCANMAT)</i> at CUTN	2012	2017	completed	UGC 12 th FYP
35.	Proposal to create a centralized High Performance Computing facility for CUTN	2012	2017	On going	UGC 12 th FYP
36.	Budget Proposal to Create a Centralized Materials Synthesis Facility	2012	2017	On going	UGC 12 th FYP
37.	Budget proposal to create a centralized instrumentation Facility	2012	2017	On going	UGC 12 th FYP
38.	Create Energy Park for Green Power at CUTN	2012	2017	On going	UGC 12 th FYP
39.	Create Academic Scholarship/Research Fellowships at CUTN level.	2012	2017	On going	UGC 12 th FYP
40.	To setup basic infrastructure for National/international research collaboration.	2012	2017	On going	UGC 12 th FYP
41.	Nanoscale Modelling of Energy-storage materials	2014	2017	completed	DST – Nanomission Program
42.	CUTN-DAE Workshop on Advances in Computational Physics 2014	2014	2014	Completed	DAE & CUTN
43.	Understanding Oxide Materials for renewable energy <i>Under Indo-Norwegian Cooperation Program (INCP)</i>	01.01.2015	31.12.2017	Completed	UGC – India & Senter for Internasjonaliser-ing av

					Utdanning (SIU) Norway
44.	Developing materials for high efficiency silicon-hybrid perovskite tandem solar cells	2017	2020	Completed	CSIR-EMR
45.	Novel Approaches to Magneto structural phase transitions in Metallic systems	2018	2022	Ongoing	Research Council of Norway
46.	Theoretical and Experimental Study and Research on Functional Materials – UTFORSK-2017	2018	2022	Ongoing	Senter for Internasjonaliser-ing av Utdanning (SIU) Norway
47	India – Norway partnership for research and education in materials for energy and environment - INTPART	2018	2021	Ongoing	Research Council of Norway
48	“Designing high efficiency thermoelectrics from high entropy half Heusler alloys using defects and disorder engineering”	2021 (10.3.21)	2023	Ongoing	DST–SERB 28, 42, 400 INR

Administrative experience:

1. Registrar (Acting) July 2014 – July 2015
2. Member – Executive Council of CUTN
3. Member – Academic Council of CUTN
4. Member – 12th FYP implementation committee
5. Chairman, Research Advisory Committee, CUTN
6. Chairman, Hostel Committee, CUTN
7. Chairman Anti-ragging committee for CUTN
8. Head, Project Cell, CUTN
9. Chairman, Examination Discipline Committee, CUTN
10. Executive Chairman, Official Language Implementation Committee, CUTN
11. Super-indent for the CUCET2014 exam, CUTN.
12. Chairman Quarters allotment committee, CUTN
13. Chairman, Grievance Redressal Committee for CUTN staff (Teaching & Administrative)
14. Member in Students Grievance committee
15. Chairman for the technical committee for purchase at CUTN
16. Chairman for the vocational training program development at CUTN.
17. As Registrar (Acting) introduced accountability and transparency in the CUTN administration by creating 6 separate administrative departments
18. Framing syllabus for 5 years integrated M.Sc. Physics program.
19. Framing syllabus for M Tech (Materials Science) program.
20. Curriculum Development for 5 years integrated M.Sc. in Materials Science & Nanotechnology and Energy & Environmental Science, CUTN.
21. Setting-up labs for 5 years integrated M.Sc. Physics program, CUTN.
22. Preparing question papers for CUCET entrance exam.
23. Selection committee member for faculty recruitment & non-teaching staffs in CUTN
24. Co-Chairperson – Library Advisory Committee, CUTN.

25. Committee member – Purchase of Modern Equipments of Mess, CUTN
26. Member - Building committee of CUTN
27. Member – Internal quality assurance cell, CUTN.
28. Member – Department promotion committee (Teaching & Nonteaching), CUTN.
29. Coordinator – Tree plantation in the Campus, CUTN
30. Coordinator – Innovation and Incubation Cell, CUTN.
31. Chairman – Quarter allocation committee, CUTN
32. Chairman, Board of Study at Department of Materials Science, CUTN
33. Member, Board of Study at Department of Materials Science, Madurai Kamaraj University.
34. Board of Study Subject Expert at Department of Bioelectronics and Biosensors, Alagappa University, Karaikudi.
35. Expert committee member, Higher secondary Physics text book Revision, SERT, Tamil Nadu.
36. Subject expert, Selection Committee for CAS promotion, The Ghandhigram Rural Institute, Gandhigram, Tamil Nadur.
37. Member in the District Environment Impact Assessment Committee for Thiruvarur and Kanyakumari Districts.
38. Program Committee member, Psik2015 conference in San Sebastián, Spain on September 2015.
39. Technical Committee member for finalizing the specifications of the equipment to be purchased for RUSA 2.0 project (Green Hydrogen based fuel cell system for day-round charging of e-vehicles), for Institute for Energy Studies, Anna University, Chennai
40. Member, Board of Study at Department of Sciences, Indian Institute of Information Technology Design and Manufacturing, Kurnool, Andhra Pradesh
41. Member of the Syllabus Sub-Committee for framing the Curriculum and Syllabi for M,Sc, Material Science (2 years), M, Phil. Physics and M.Phil Crystal Science to be offered under R-2023 by the Physics Departments of Anna University, Chennai.
42. Board of study member for B.Voc program for the Community college, CUTN.
43. Member of standing purchase committee for procurement of Goods and Services, 2023-24, CUTN.

EXTENSION AND CO-CURRICULAR ACTIVITIES

- Coordinated a Lab2Moon project to send cyanobacteria extremophiles in a bioreactor to Moon to study photosynthesis process at Moon environment through SpaceX project and competed till last round and prototype biochemical reactor was build.
- Appointed paper setter to recruit Group A service in a southern state of India in 2022 (confidential).
- Setup question papers for MSc(Materials Science) at Alagappa University, Karaikudi.
- Invited experts (national & international) in advanced research field to organize department seminars
- Student counselling
- Actively involved in bringing internet and Wi-Fi facilities in CUTN.
- Organized educational tour to IMSc students to advance research labs
- Adjunct professor in University of Oslo, Norway work during vacation period : Teaching a course + setting up computational lab – give project work – evaluating it from 2010 onwards
- Given invited talks in Department of Tamil
- Given invited talks to students in Science day meeting at neighboring school in Thiruvarur, INDIA
- Chief guest and distributing prizes in Cultural and Sports Programmes
- Helped students to get summer internships and PhD position abroad.

- Special efforts made to clear the canals and make fencing to protect the campus from grazing animals in CUTN
- Participated cycle rallying in Swachh Bharat Abhiyan held in CUTN
- Working late hours to mentor PhD and Master students (5 pm to 9 pm , daily)
- Arrange group weekly seminar and also department seminars.
- Spent substantial amount of time to design interiors of buildings for the School of Basic and Applied Sciences.
- Planted trees (3000) around the Professors/staff quarters & campus in CUTN

OTHER RESEARCH ACTIVITIES

Supervision:

Supervision	Candidates
Post-doctoral Fellows	<ol style="list-style-type: none"> 1. Dr. Smagul Zh. Karazhanov – Solar-energy materials 2. Dr. P. Vajeeston – Nanophases of hydrogen-storage materials 3. Dr. R. Vidya – Magnetic thinfilms & Defects in semiconductors 4. Dr. Maria Iozzi – Search for p-type transparent-conducting oxides 5. Dr. Li Ming – DFT on metal-organic frameworks 6. Dr. Nupinderjeet Kaur – Hydrogen-storage materials 7. Dr.Krishanmoorthy – Novel Magnetism – NPDF . 8. Dr.S.Kiruthika – Hybrid solar Cell – Research Associate.
Master students	<ol style="list-style-type: none"> 1. Anu Maria Aguestine, Predicting superhard Materials, CUTN, 2015 Now doing PhD at CUTN. 2. Varunaa, Phase stability studies and alkali metal hydrides, CUTN, 2015. 3. Espen Sagvolden – Effect of exchange-correlation functionals on charge density (later did his Ph.D under Prof. John Perdew at Tulane Univ. USA)-2007, Now faculty at UiO). 4. Beate Larsen – Studies on novel metal-organic frameworks –2012. 5. K. Syam Kumar – CO₂ storage in MOFs 2016, Completed PhD at Ireland. 6. H.J. Karthick, - Modelling Mg-based hydrogen storage Materials, 2016. 7. K.G. Geo Sunny, - Developing efficient electrodes for Li-ion batteries 2016 Now doing PhD at CUTN. 8. Ansu Elsa Ninan, - Non Si-based solar cell materials 2016. 9. Mukesh Kumar Choudhary – Search for potential thermoelectric materials 2016, Now doing PhD at CUTN. 10. Alok Mishra - Phosphorene-AsP Heterostructure as a Potential Excitonic Solar Cell Material - A First Principle Study (2017). 11. C. Vivek- Ab Initio Modelling of New Cathode Material for Li-Ion Batteries (2017) Now doing PhD at UK. 12. K.V. Varun, Theoretical Investigation of Alkaline Earth-Ammine Borohydrides (2017). 13. R. Prameela, Titanium Substituted Magnesium Hydride for Hydrogen Storage Applications (2017). 14. Sharath V - Electronic Structure and Thermoelectric Properties of Half-Heusler 8 VEC Compounds;From Ab Initio Calculations.(2017) Now doing PhD at IIT. 15. Y. Ramya Koteswari- Computational modelling of magnetoelectric materials (2018). Now working at IIT, Madras.

16. M. Kavitha- Polyanionic cathode materials for Li-ion battery (2018).
17. Puvinila- Computational study of engineered 2D materials for photocatalysis (2018).
18. P Sri Harsha- Computational study of engineered 2D materials for photocatalysis, Now doing Ph.D at University of Iceland (2018).
19. Suresh .R- First principles study of novel intermediate band solar cell materials $\text{NaAl}_{1-x}\text{S}_2\text{Ti}_x$, (2019) Now doing PhD at CUTN
20. Arjun R Krishnan- Ab initio modelling of multiferroic materials, (2019).
21. Gopika G Pillai- Ab initio calculations of novel oxide based solar cell materials, (2019).
22. Rashid Rafeek. V- First principle study of V_2O_5 and MoO_3 with oxygen vacancy as cathode material for magnesium batteries, (2019).
23. Archa Santhosh- Two dimensional Mxene nanosheet for future hydrogen storage applications: A first principal study, (2019) Now doing PhD at Germany
24. T.A.Anaka Thermoelectric properties of Cs_3Bi and K_3Bi (2020)
25. G.Greeshma, First-Principle study of pnictide compounds for photovoltaic applications (2020)
26. R.Geethanjali, Designing AB type binary thermoelectric materials (2020)
27. S.Anusree, Two-dimensional SnH and GeH for photovoltaic applications – A first principle study (2020).
28. Darshana Sudheer, First principle modelling of Bismuth based multiferroic materials (2020)
29. K.Vaigal, $\text{K}_2\text{Sn}_2\text{ZnO}_4$ for photocatalytic water splitting: A first principle study (2020)
30. C.V.Vishnu Prasad, First principle study of $\text{Na}_2\text{CuC}_2\text{O}_6$ as a cathode materials for sodium ion batteries (2020)
31. P.Sundar, First-principles study on complex metal hydrides Na_2MgMH_7 (M=Sc,Ti,V,Cr,Mn,Fe,Co,Ni,Cu) based on 3d transition metal series for hydrogen storage applications (2020)
32. S.K.Aravind, Designing new complex hydrides based on transition metals for hydrogen storage applications (2020)
33. Aasif Majeed, First Principle Study of Sn doped V_2O_5 with Oxygen Vacancy as Cathode Material for Magnesium Batteries (2021)
34. Amal Raj V, Ab-initio study of novel photocatalytic material: $\text{K}_2\text{Sn}_2\text{ZnO}_4$ (2021)
35. Irfan Ahmad Lone, In-Silico study of novel intermediate band solar cell material: $\text{MgSn}_{(1-x)}\text{V}_x\text{P}_2$ (2021)
36. Ravi Kaushik, Design of Bi^{+3} Based Magnetoelectric Multiferroics (2021). Now doing PhD at Italy.
37. K.Amritha, An ab initio Study of Designing New Ternary Transition based Hydrides for Hydrogen Storage Applications (2022) Now at IIT, Guwahati, India.
38. R.Abhinaya, Phosphorous Based Ternary Compounds for Solar Cell Applications – An ab initio Study (2022)
39. Munavvar Husain, Designing New Complex hydrides based on Transition Metals for Hydrogen Storage Applications (2022) Now doing PhD at Warsaw, Poland.

	<p>40. S.Sneha, Nontransition Metal Based 2D Materials for Optoelectronic applications: An <i>ab initio</i> Study. (2022) Now doing PhD at IIT, Tirupati.</p> <p>41. V. Clement Paulson, Data Driven Approach for Accelerated Band Gap predication and Novel Materials Discovery. (2022) Now doing PhD at Austria.</p> <p>42. P.S.Amal Mathyas, Firtst Principles Investigation of $K_2Mn(CO_3)_2$ As A Novel Polyanionic Cathode Material for Potassium Ion Battery (2023)</p> <p>43. K.K. Ashiq Muhammed, Two-Dimensional BP-GMO Heterostructure for Photocatalytic Water Splitting : A First Principles Study (2023)</p> <p>44. V. Abhiram, First Principles Studies of Re_2Sn as a Thermoelectric Material, (2023)</p> <p>45. Amrendra Kumar Tiwari, High Capacity Hydrogen Storage Materials based on Transition Metal-based Complex Hydrides $NaMgTH_6$ (T=Sc-Cu) : An Ab Initio Study (2023)</p> <p>46. R.Nirmal Kumar, Prediction Potential Hydrides for the Hydrogen Storage from Oxides via Machine Learning (2023).</p> <p>47. Shubhasis Behera, Ab-initio Modelling of V_2C and V_2N based MXene for Hydrogen Storage Applications (2023)</p>
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List of PhD students supervised/under supervision:

S. No	Name of PhD	Title of Thesis	Supervising level	Year of completion
1.	Ponniah Vajeeston	Theoretical Modelling of Hydrides	Co-Supervisor	2004
2.	Chris Erik Mohn	“Computational studies of the potential energy hypersurface of disordered systems — linking structure, energetics and dynamics”	Co-supervisor	2005
3.	Laila Offernes	Bonding and physical properties of half-Heusler phases	Main Supervisor	2007
4.	Arne Klaveness	Quantum-mechanical modeling and complex hydrides	Main Supervisor	2007
5.	Rune Søndena	Connectivity of polyhedra in $AMnO_3$ (A=Ca, Sr, Ba) and AB_2 (A=Si, Ge; B=S, Se)	Co-supervisor	2007
6.	Ashwin Kishore M.R	Tailoring the Electronic Band Gap and Band Edge Positions of C_2N Monolayer for Photocatalytic Water Splitting: A First Principles Study	Main Supervisor	2018
7.	Lokanath Patra	Theoretical investigation on layered magnetic oxides	Main Supervisor	2019
8.	S.Kiruthika	Design of Hydrogen storage materials from first principles	Main Supervisor	Thesis submitted
9.	P.D.Sree Devi	Predicting nonsilicon based materials for high efficiency solar cells.	Main Supervisor	Thesis submitted
10.	A.Ramesh	Graphene based nanostructures of hydrogen storage.	Co-supervisor	2018

11.	Anu Maria Agustine	Nanoscale modelling of materials for Li-ion batteries.	Main Supervisor	Started 2015
12	R.Varunaa	Nanoscale modelling of hydrogen storage materials.	Main Supervisor	2020
13	Mukesh Choudary	Design Thermoelectric intermetallics.	Main Supervisor	Thesis submitted
14	Vishnu Sudarsanan	Develop high efficiency electrodes for Li-ion batteries	Main Supervisor	Started 2016
15	Suresh R	Designing Magnetocaloric Materials for Efficient refrigeration.	Main Supervisor	Started 2019
16.	Santy M Thomas	2D Materials for photocatalytic water reduction for H ₂ production.	Main Supervisor	Started 2019
17	Gowri Shankar	Thermoelectrics from maximum entropy Alloys.	Main Supervisor	Started 2022

Refereeing articles for following International Journals:

1. Journal of American Chemical Society, 2. Physical Review Letters, 3. Physical Review B, 4. Journal of Applied Physics, 5. Applied Physics Letters, 6. Journal of Solid State Chemistry, 7. Computational Materials Science, 8. Surface Science, 9. Journal of Molecular Structure, 10. European Journal of Inorganic Chemistry, 11. The Journal of Physical Chemistry, 12. Journal of Alloys and Compounds, 13. International Journal of Hydrogen Energy, 14. The European Physical Journal B, 15. Journal of Physics Condensed Matter, 16. Physica B, 17. Physics Letters A, 18. Phase Transitions, 19. Journal of Physics and Chemistry of Solids, 20. Materials Science and Engineering B, 21. Physica Status Solidi B, 22. Chemistry of Materials, 23. Advanced Materials, 24. Physica Scripta, 25. Solid State Sciences, 26. Journal of Zhejiang University-SCIENCE A, 27. Angewandte. Chemie. International Edition, 28. Nanotechnology, 29. Nature Communication, 30. Euro Phys. Lett, 31. J. Magn. Mag. Mater., 32. Materials Sciences and Applications, 33. Materials Science in Semiconductor Processing, 34. Progress in Natural Science: Materials International, 35. Journal of Photochemistry & Photobiology, B: Biology, 36. Advances in Condensed Matter Physics, 37. Optik – International Journal for Light and Electron Optics, 38. Journal of Chemical Physics, 39. International Research Journal of Pure and Applied Chemistry, 40. Nature-Scientific Reports, 41. Nanoscale Advances, 42. Catalysis Today, 43. Inorganic Chemistry Communication, 44. Materials Research Letters, 45. Pramana – Journal of Physics, 46. Journal of Materials Science, 47. Solid State Communication, 48. Surfaces and Interfaces, 49. Separation and Purification Technology, 50. Computational Condensed Matter, 51. Journal of Materiomics, 52. Chemical Physics, 53. Bulletin-of-Materials-Science, 54. Recent Patents on Nanotechnology, 55. Computational Theoretical Chemistry, 56. Composites Part B.

Book Refereeing:

1. Reviewed the book titled “*Advances in Material Science and Application Tale of Two Stalwarts Face to Face Bulk (Silicon) Vs Nano (Graphene) Vol. I & II*, Cambridge University press (2022).
2. Reviewed the book titled “*Intelligent Materials by Design*, Cambridge University press (2023).

Editorial Boards:

1. Chairman of the Editorial board for World Journal of Condensed Matter Physics, Scientific Research Publishing (www.scirp.org) 5005 Paseo Segovia, Irvine, CA 92603-3334, USA
2. Editorial Advisory Board member for The Open Condensed Matter Physics Journal (ISSN: 1874-186X) www.bentham.org/open/tocmpj .

Refereeing research proposals for

1. National Science Foundation (NSF), USA
2. Department of Energy (DOE), USA
3. Department of Energy-Basic Energy Sciences (DOE-BES), USA.
4. Indian Institute of Technology, Kanpur, India
5. Solar Energy Research Initiative (SERI), DST, India
6. Preludium founding scheme of National Science Center in Poland
7. Research Innovation Grant of Khalifa University of Science & Technology (KU), Abu Dhabi, United Arab Emirates (2022).
8. Kerala Biotechnology Commission, Kerala Government (2022).
9. KSCSTE-PDF scheme for Kerala State Council for Science, Technology and Environment (2022).
10. UGC, India Fellowship and Research Grants for Fellowship for Superannuated Faculty Members; Research Grant for In-Service Faculty Members; Dr. D.S. Kothari Research Grant for Newly Recruited Faculty Members & Dr. S. Radhakrishnan Post-Doctoral Fellowship.
11. Evaluation committee member to review the performance of UGC-FRP faculty.

Ph.D Examiner:

1. J.Beena, Manonmaniam Sundaranar University, Tirunelveli, Tamil Nadu (June 23)) thesis entitled "Studies on Semi Organic Family of Single Crystal".
2. V.R.Manjula, Osmania University, Hyderabad, Telangana (January 2023) thesis entitled "Thermography Analysis of defects in CFRP composites".
3. Maya Mathew, Payyannur College, Kannur University, Payyanur, Kerala (June 2022) thesis entitled "Optoelectronic Applications Oriented Synthesis and Characterization of Binary, Ternary, and Quarternary Copper and Lead based Quantum Dots".
4. Ikram Un Nabi Lone, Crescent Institute of Science and Technology, Chennai March 2020 thesis entitled "A DFT Study On Half Metallic Ferro-Magnetism In Doped Chromium Phosphide: First Principles Calculations"
5. Giruba M, Dr.M.G.R. Educational and Research Institute, Maduravoyal, Chennai, (August 2021) thesis entitled "Structural, Electrical, Optical And Antimicrobial Studies Of Undoped and Ag, Cu Doped ZnO Based Nanomaterial for Optoelectronic Devices"
6. Akshaya Devi E, Indira Gandhi Centre for Atomic Research, Kalpakkam, India, June 2021 thesis entitled "First-principles study of energetics of atomic defects and stability of B1- type oxides in bcc ferromagnetic iron"
7. Alaka Panda, Indira Gandhi Centre for Atomic Research, Kalpakkam, India, July 2020 thesis entitled "Mössbauer Studies on Some Fe-based Multiferroic Materials".
8. J. Celina Selvakumari, Manonmaniam Sundaranar University, Thirunelveli, November 2018, thesis entitled "Green Synthesis, Characterization and Energy Storage application of RGO and Metal Oxide Nanoparticles".
9. Naga Vekateswara Rao, CLRI, Chennai, October 2018, thesis entitled "Computational Studies on the Design and Development of Carbon based Novel Two Dimensional Dirac Materials".
10. Mr.J.Karthikeyan, CECRI, Karaikudi April 2018, thesis entitled "First Principles Calculations on Structural Stability and Physicochemical Properties of Mo-S Nanostructures"
11. Mr.J. Bennet, Department of Physics, Anna University, March 2018, thesis entitled Investigation on Structural, Optical, Magnetic and Dielectric Properties of Spinel AFe_2O_4 ($A=Co, Mg, Mn, Zn$ and Cu) Ferrite.
12. Mr.S.Vadivelan, Department of Physics, Anna University, March 2018, thesis entitled "Synthesis and Characterization of Pristine and Cr, Co, Ni, Zn & Sr Doped Nano Barium Ferrites"
13. Mr. Iyyappa Rajan P, VIT University, Chennai, India, February 2018, thesis entitled "Computational Studies on Electronic and Magnetic Properties of Multiferroic Materials"
14. Mr. N.Karthikeyan, Anna university, Tiruchirappalli, India, August 2017 thesis entitled "FT-IR and FT-Raman vibrational investigation on biologically Active molecule using computational calculation".
15. R. Jegadeesan, Bharathidasan University, India, March 2017 thesis entitled "Structure, Bonding, Reactivity, and spin-crossover in Organometallic Complexes involving late transition metals"

16. S. Selva Chandrasekaran, CECRI, India, March 2017, thesis entitled "Theoretical investigation on Surfaces and Interfaces of Rare-earth based exchange-sprint-magnet".
17. G. Umadevi, Bharathiar University, India, April 2011, thesis entitled "Synthesis and Characterization of Protonic Acids Doped Polyaniline by Electrochemical and Chemical Oxiation Methods".
18. K.Tamilselvan, Bharathiar University, India, February 2012, thMr.esis entitled "Preparation, Characterization, and Performance analysis of ZnO thin film based temperature sensor".
19. Mikael Råsander, Uppsala University, Sweden June 2010, thesis titled "Theory of transition-metal carbides-including carbon diffusion, graphene, and magnetic carbides"
20. S. Palanisawamy, Bharathiar University, India, thesis titled "Growth and Characterization of some semi-organic non-linear optical materials". January 2010
21. Alexei Grechnev, Dept. of Physics, Uppsala University, April, 2005. Ph.D thesis titled "*Theoretical Studies of Two-dimensional Magnetism and Chemical Bonding*".
22. David Andersson, Dept. of Materials Science and Engineering, Royal Institute of Technology, Sweden in April, 2007. Ph.D thesis titled "*From the Electronic Structure of Point Defects to Functional Properties of Metals and Ceramics*".

Member:

- External Expert in the Committee constituted to frame the leave rules for Indian Association for Cultivation of Science, Kolkata (2023).
- Evaluation committee for the FUNMAT- related projects at University of Oslo, Norway.
- Member Assessment Committee Report For Upgradation from JRF To SRF at CSIR-Central Electrochemical Research Institute, Karaikudi
- Doctoral Committee Member for Mr.Keerthivasan at SSN College of Engineering, Chennai
- Selection Committee member for faculty recruitment at Department of Physics, Central University of Tamil Nadu.
- Selection Committee member for nonteaching staff recruitment in Central University of Tamil Nadu.
- Doctoral Committee Member for Mr.N.D.Senthil Ram at SRM Institute of Science and Technology, Kattankulathur.
- Recruitment board for selecting PhDs and Postdocs at University of Oslo, Norway
- **Steering Committee member of ESF- Ψ_k Network** and Co-ordinator of Norwegian node (ESF- Ψ_k represented by 25 EU countries with nearly 1000 scientists from around the globe).
- American Chemical Society, USA, since 2019
- Materials Research Society, Singapore, since 2003
- Theoretical Physics Seminar Circuit, 1995, India
- Active participant in WIEN2k, VASP, PWSCF, SIESTA, and ABINIT mailing lists.

TEACHING EXPERIENCE

- ❖ I have been teaching (i) *Electricity and Magnetism*, (ii) *Atomic and Molecular Physics*, (iii) *Solar Energy and its Applications*, (iv) *Semiconductor Physics*, (v) *Properties of Materials*, (vi) *Condensed Matter Physics* and (vii) *Computational Materials Science*, (viii) *Advanced Computational Condensed Matter Physics*, (ix) *Nanomaterials & Nanotechnology*, x. *Synthesis and Characterization of Advanced Functional Materials*, xi. *Synthesis and Characterization of Materials* courses for Integrated MSc, MTech, students and PhD students at the Central University of Tamil Nadu, India since 2012.
- ❖ I have been involved in establishing the labs for IMSc students and also teaching in the Electricity and Magnetism Lab, Modern Physics Lab & Condensed Matter Physics Lab.
- ❖ I have lectured a 5-credit intensive graduate course on *Ab-initio Modelling of Solar Energy Materials* at University of Oslo in spring semester from 2010 onwards comprising of 30 hours lecturing and 30 hours hands-on training in the computer lab. The course lectures can be found at <http://folk.uio.no/ravi/FME2011/lectures/> and tutorial notes at <http://folk.uio.no/ravi/FME2011/tutorial/>

- ❖ I have lectured a 4-credit intensive graduate course on Computational Materials Science – Principles and Practices in the Autumn semester for the years 2002-2011 at University of Oslo, Norway for PhD and Master students.
- ❖ Framed syllabus for the five year integrated MSc program in Physics at the Central University of Tamil Nadu.
- ❖ Developed curriculum for the two year MTech program in *Materials Science* and also *Energy and Environmental Science*.

The Courses Taught in the University Level:

S.No	Course title	Credit	Name of the Institution/University	Year	Course link
1	Computational Materials Science – Principles and Practices	4	University of Oslo, Norway	2002-	https://folk.universitetetios.no/ravi/cutn/ccmp.html
2	Ab-initio modelling of Solar Energy Materials	5	University of Oslo, Norway	2010-	http://folk.uio.no/ravi/FME2011/lectures/
3	Atomic and Molecular Physics	3	Central University of Tamil Nadu	2012-	https://folk.universitetetios.no/ravi/cutn/atomicphy.html
4	Solar Energy and its Applications	3	Central University of Tamil Nadu	2012-	https://folk.universitetetios.no/ravi/cutn/solar.html
5	Electricity and Magnetism	3	Central University of Tamil Nadu	2013-	https://folk.universitetetios.no/ravi/cutn/elec_mag.html
6	Semiconductor Physics	4	Central University of Tamil Nadu	2013-	http://folk.uio.no/ravi/cutn/teaching.html
7	Condensed Matter Physics	4	Central University of Tamil Nadu	2013-	https://folk.universitetetios.no/ravi/cutn/cmp.html
8	Properties of Materials	4	Central University of Tamil Nadu	2014-	https://folk.universitetetios.no/ravi/cutn/pmat.html
9	Computational Condensed Matter Physics	4	Central University of Tamil Nadu	2015-	https://folk.universitetetios.no/ravi/cutn/ccmp.html
10	Advances in Computational Materials Science	2	Central University of Tamil Nadu	2016-	https://folk.universitetetios.no/ravi/cutn/acms.html
11	Nanomaterials and Nanotechnology	4	Central University of Tamil Nadu	2016-	https://folk.universitetetios.no/ravi/cutn/nmnt.html
12	Synthesis and Characterization of Advanced Functional Materials	4	Central University of Tamil Nadu	2018-	http://folk.uio.no/ravi/cutn/teaching.html

ORGANIZER

- Convener of the International Summer School on “Materials Informatics & Biophotonics for Medical and Energy Research (InSuMMER-2023) with 60 participants and 23 speakers) held at Anna University, Chennai, India on 29 May to 16 June 2023.
- Convener of the Indo-Norway workshop on “Functional Materials for Energy Technology (FMET-2019) (with 200 participants) held at Central University of Tamil Nadu, Thiruvarur, India on 23-24 September 2019.
- Convener of the International Conference on “Advances in Functional Materials (ICAFM17)” (<http://folk.uio.no/ravi/icafm17>) (with 500 participants) held at Anna University, Chennai, India on 6-8, January 2017.
- Convener of the workshop on “Light – Matter interaction in Science” (SPECTRUM2015) (<http://folk.uio.no/ravi/cutn/spectrum15/>) (with 220 participants and 10 speakers)) held at Central University of Tamil Nadu, India on 30-31, October 2015.
- Coordinator for the CUTN-DAE workshop on Advances in Computational Materials Science, 2015 (ACMS2015) <http://folk.uio.no/ravi/ACMS2015/> (with 150 participants, 18 speakers) held at Central University of Tamil Nadu, India on 23-25, April 2015.
- Organizer of “Mini Symposium on Advances in Solar Thermal Technologies” at Department of Chemistry, University of Oslo, Norway on 11 June 2014.
- Convener of workshop on “Advances in Computational Physics 2013” (<http://folk.uio.no/ravi/ACP2013>) (with 150 participants) at Central University of Tamil Nadu from 14-16, February, 2013.
- Organizer, Research School on Computational Materials Science for Energy Technology 2009 (<http://folk.uio.no/ravi/CMS-ET2009>) between April 28-29, 2009 at Center for Materials Science and Nanotechnology, University Of Oslo, Norway.
- Convener of “International workshop on computational materials science from Full potential method” (with 100 participants) held from December 12-16, 2011 as a parallel event in the ICAM2011 at PSG College of Technology, Coimbatore, India.
- Co-ordinator for the "Indo-Norwegian Workshop on Solar Energy Materials and Applications" (with 120 participants) held from December 13-15, 2011 as a parallel event in the ICAM2011 at PSG College of Technology, Coimbatore, India.
- Convener for the “Indo-Norwegian workshop on Materials for Hydrogen Storage and Fuel Cells” (with 100 participants) held from December 13-15, 2011 as a parallel event in the ICAM2011 at PSG College of Technology, Coimbatore, India.
- Convener for the " Indo-Norwegian Satellite Meeting on Advances in Solar Cell Materials & Technology" (with 120 participants) on 17 December 2011, Madurai Kamaraj University, Madurai, India.
- Co-chairman for the International conference on advanced materials (ICAM2011) (with 500 participants) held from December 12-16, 2011 at PSG College of Technology, Coimbatore, India.
- International Advisory Committee member for the International conference on Materials Science Research and Nanotechnology and chaired 2 sessions, ICMSRN2008, Mother Teresa University, Kodaikanal, India February 27-29, 2008.

Organizing committee members in the following conferences/workshop:

- 8th European Conference on Solid State Chemistry, Oslo, Norway, 4-7 July (2001)
- 28th Journees des Actinides, Uppsala, Sweden, May 14-16 (1998)
- International Workshop on Electronic structure calculations and properties of Materials, Anna University, Chennai, India, Nov. 16-21 (1992).
- National Symposium on Band structure and its applications to the study of properties of Materials, Anna University, Chennai, India, Feb. 13-15, (1990).
- Organized periodic group meetings in the research groups where I have worked.

SCIENTIFIC VISITS TO VARIOUS INSTITUTIONS

1. Prof. T. Venkatesan’s Nanocore Group at National University of **Singapore**, 24-30 Sept. 2013.

2. Prof. Ole Krogh Andersen, Max-Planck-Institut fuer Festkoerperforschung, Stuttgart, **Germany** from 21-23 November, 2010 for scientific collaboration.
3. Prof. Vikram Jayaram's group & Prof. Chandan Das Gupta group at IISc, Bangalore, **India** from 26-31, July 2010 for scientific interaction.
4. Prof. Shobhana Narasimhan's group at JNCASR, Bangalore, **India** from 12-14 March 2008 for scientific collaboration.
5. Prof. Manuel Richter's group at Leibniz Institute for Solid State and Materials Research (IFW), Dresden, **Germany** from 26 May- 01 June 2007 to use FPLO code.
6. Prof. Yia-Chung Chang's group at Research Center for Applied Sciences, Academia Sinica, Taipei, **Taiwan** from 15-21, November 2006.
7. Prof. Z. Jirak's group at Institute of Physics ASCR, Prague, **Czech Republic** from 30 Aug. 04. Sept. 2004 to study Spin, Charge and Orbital Ordering in perovskite like oxides.
8. Prof. Olle Eriksson's Condensed Matter Theory Group, Uppsala University, **Sweden** from 18-27 June, 2001 to perform force minimization and parallel computation using FPLMTO method.
9. Prof. Claudia Ambrosch-Draxl group, Institut f. Theoretische Physik, University of Graz, **Austria** from Aug. 7-21, 2000 to investigate the Raman spectra of superconductors.
10. Condensed Matter Theory Group, Uppsala University, **Sweden** from 02 Dec 1999 to 12 Jan, 2000 for doing non-collinear spin density functional calculations for perovskite oxides.
11. Prof. Jürgen Hafner, Institut fuer Theoretische Physik and Center for Computational Materials Science (CMS), Technische Universitaet Wien, **Austria** from 07-09 April 1999 to use VASP.
12. Prof. Helmer Fjellvåg group, Department of Chemistry, University of Oslo, **Norway** from 28-30 Sept. 1998 for a project planning meeting.
13. Prof. Claudia Ambrosch-Draxl group, Institut f. Theoretische Physik, University Graz, **Austria** from 08-20 June, 1998, wrote a proposal on Electronic Structure Studies of Ferroelectrics.
14. Prof. Karlheinz Schwarz group, Vienna University of Technology, Computational Quantum Theory Group, **Austria** from 01-11 July, 1997.

Academic Staff College Orientation/ Refresher Course attended:

Name of the Course/ Summer School	Place	Duration	Sponsoring Agency
Training programme in Appreciation Course In Heat Treatment of Materials	Guindy, India	06-06-1988 to 01-07-1988	Advanced Training Institute. Directorate General of Employment and Training, Ministry of Labour-Govt. of India
Basic Course in Swedish	Folkskolan, Uppsala, Sweden	3 Months (evening) in Spring 1997	Uppsala University, Sweden
Basic Course in Swedish	Aara skolen, Uppsala, Sweden	3 Months (evening) in Autumn 1997	Uppsala University, Sweden
Basic course in Norwegian for Foreigners Level 1	UiO, Oslo, Norway	3 months in Autumn 2009	University of Oslo, Norway
Basic course in Norwegian for Foreigners Level 2	UiO, Oslo, Norway	3 months (evening) in Spring 2010	University of Oslo, Norway
Basic course in Norwegian for Foreigners Level 3	UiO, Oslo, Norway	3 months (evening) in Autumn 2010	University of Oslo, Norway

Online Orientation Training Programme for Mentors from Higher Education Institute	NITTTR, Chennai	1 st to 10 th February, 2021.	Ministry of Education, Government of India
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Invited talks in the National and International level

S.No	Title	Name of Event	Place of The Event	Date and Year
1.	<ul style="list-style-type: none"> i. Basics of Density functional calculations 1 ii. Basics of Density functional calculations 2 iii. Design High Efficiency Hydrogen Storage Materials iv. Efficient Solar Cell Materials from ab initio Calculations v. Modelling of Magnetic oxides vi. Magnetoelectric Multiferroics 	International Summer School on "Materials Informatics & Biophotonics for Medical and Energy Research (InSuMMER-2023) Totally 6 lectures with each lecture 1.5 hrs.	Department of Medical Physics, Anna University, Chennai, India	29 May to 16 June 2023.
2.	Materials for Energy Technology from Computational Approach for Sustainable Energy	International Workshop on Quantum Mechanical Modelling of Materials by Quantum Espresso	Parveen Singh Institute of Technology, Uttar Pradesh, India	March 15-19, 2023
3.	Designing Functional Materials for Green Energy Generation	DST – SERB Sponsored online Workshop on Electronic Structure Calculations for Molecules and Materials	Bharathiar University, Coimbatore, India	April 17, 2023
4.	Designing Functional Materials for Green Energy Storage	DST – SERB Sponsored online Workshop on Electronic Structure Calculations for Molecules and Materials	Bharathiar University, Coimbatore, India	April 21, 2023
5.	Ab- Initio Studies on Functional Materials for Renewable Energy Technologies	International Conference on Recent Trends in Applied Science and Technology (ICRTAST-23)	Madras University, Chennai, India	March 16-17, 2023
6.	Efficient Energy Generation, Conversion and Storage Materials from Computational Approach	International Conference on Advanced Novel Materials in Multi- Disciplinary Perspectives (ICAMP '23)	St. Joseph's College of Arts & Science, Cuddalore, India	3 & 4 th March 2023.
7.	Efficient Energy Generation and storage materials for green energy technologies from Computational Approach	3rd International Symposium on Modeling of Crystal Growth Processes & Devices (MCGPD-2023)	SSN Research Centre, SSN Institutions, Chennai, India	06-08 March 2023.

8.	Advanced Functional Materials for Green Energy Generation.	Refresher course on “Recent Advances in Physics of Materials	School of Physics, Madurai Kamaraj University, Madurai	7th Oct – 20th Oct 2022
9.	Current Trend in Solar Thermal Technologies	Refresher Course In Physics, Batch – Xxiv	Nuclear Physics Department, University of Madras, Chennai 25.	9-22 September 2022.
10.	Designing Functional and Nanomaterials for Renewable Energy Technologies	Refresher Course in Physics & Nanotechnology,	Bharathiar University, Coimbatore - 46	08-14 September 2021
11.	Density of States effects on optical processes in solids - an <i>ab initio</i> study	Colloquium on Light-matter interaction at nanoscale	Srinivasa Ramanujam Institute of Basic Sciences, Kottayam	22-25 July 2021.
12.	Designing High Efficiency Materials for Renewable Energy Technologies	International Symposium on Modeling of Crystal Growth Processes and Devices (MCGPD - 2021)	SSN Research Center, Chennai, India	05-07 July 2021
13.	Designing Advanced Functional and Nanomaterials for Energy Technologies	2nd Indo-Korea Virtual Conference on Development of Advanced Materials for Future Technologies (DAMFT - 2021)	VIT Chennai, India	14 – 15 May 2021
14.	Grand Challenges for Sustainable Development	National Science Day Celebration 2021	CUTN, Dept. Phys, Thiruvarur	26.2.2021
15.	Hydrogen Economy for Mitigation of Climate Change	UGC Stride Free Virtual 10 Days FDP On “Mitigating Climate Change	Central University of Tamil Nadu, Thiruvarur, India	26th April To 6th May 2021
16.	Spectroscopic Studies on Functional Materials from first principles calculations	National Photonics Symposium NPS-2020	International School of Photonics, CUSAT, Cochin, India	27-29 February 2020
17.	Designing Advanced Functional Materials for Sensor Applications	Nanomaterials Driven Advances in Chemical and Biosensors (NanoSe2019)	Alagappa University, Karaikudi, India	27-29 November 2019.
18.	Design high efficiency cathode for Li and non-Li based batteries.	Key note address at National Conference on Transition Metal based Sodium Ion Batteries (SIBs) for Ultrafast Energy Storage Systems	Dr. N.G.P. Institute of Technology Coimbatore, India	13 November 2019
19.	Design Functional Materials for Renewable energy technologies	Indo-Norway workshop on Functional Materials for Energy Technology (FMET-2019)	SCANMAT, Central University of Tamil Nadu, India	23-24 September 2019.

20.	First principles investigation on functional materials for energy technology	International Seminar on Materials for Energy and Environmental technologies.	University of Oslo, Norway	20-22 May 2019
21.	Design functional materials for energy and sensor applications	National Conference on Advanced Materials for Sustainable Energy and Sensors (NCAMSES-2019)	Department of Physics, Alakappa University, Karaikudi	20-22 March 2019
22.	Develop Functional Materials for energy harvesting from <i>Ab initio</i> Calculations	International symposium on Modelling of Crystal Growth Processes, and Devices (MCGPD-2019)	SSN Institutions, Chennai	26-28, February 2019
23.	Design Multifunctional Materials from <i>Ab initio</i> Calculations	International conference on Advanced Materials for Clean Energy and Health Applications (AMCEHA 2019)	University of Jaffna, Sri Lanka	6-8 February, 2019
24.	Design Higher Efficient thermoelectric Materials using Multinary Alloys for sustainable energy	Two day Symposium on Thermoelectric Materials, Devices and Systems	PSG COLLEGE OF TECHNOLOGY, COIMBATORE	10-11 December 2018
25.	Design advanced functional Materials from <i>Ab initio</i> Calculations.	CSIR sponsored summer workshop on "Modelling and Simulations in Materials Science and Engineering (MSME2018)	Department of Physics, Sathyabama Institute of Science and Technology	18-22 June 2018.
26.	Design Complex Multiferroics with giant magnetoelectric coupling	Annual Meeting on Physics of Strongly Correlated Electron Systems (PSCES2018)	Indian Institute of Technology, Mandi, Himachal Pradesh, India	02-04 April 2018.
27.	Characterization of Materials from First Principle Calculations	Synthesis, Characterization and Applications of Nano Materials (ISTC-SCAN-2018)	Department of Chemistry of Sri Jai Narain (P.G.) College, Lucknow	6-12 March 2018
28.	Design functional materials for energy harvesting	APAM lecture	Department of Physics, Barathidasan University, Trichy	13 Feb 2018
29.	Recent Advances in solar thermal technologies for energy Harvesting	Department Seminar	Department of Physics, CUTN	21 July 2017
30.	Understanding oxide materials for Renewable Energy	INCP Midterm Review Workshop	UGC, Delhi	4 July 2016
31.	Develop Penta/Exascale computational resources for scientific computing	Indo-Norwegian ICT Workshop	IIIT, Hyderabad, India	21-23 June 2016
32.	Bandgap Engineering	Summer Training Program in Physics	Department of Nuclear Physics, University of	8 June 2016

			Madras, Chennai, India	
33.	Research Methodologies for Scientist	Workshop on IP awareness and Research Methodologies.	Department of Mathematics, Central University of Tamil Nadu.	16 October 2015
34.	Indian Science and Challenges	Workshop on IP awareness and Research Methodologies.	Department of Mathematics, Central University of Tamil Nadu.	16 October 2015
35.	Recent Development in Solar Thermal Technologies	Mini Symposium on Advances in Solar Thermal Technologies	Department of Chemistry, University of Oslo, Norway	11 June 2014.
36.	Bulk and Nanophases of Hydrogen Storage Materials from Computational Modelling	National Seminar on Advances in Materials Science 2014 (NSAM2014)	Mononmaniam Sundaranar University, Thirunelveli, India	28,29 September 2014.
37.	Ground State and Excited state properties from DFT	Meeting on Physics from Electronic Structure	Institute of Mathematical Sciences, Chennai, India	16 April 2014
38.	Characterization of Materials Properties from abinitio Calculations,	Materials Characterization Technique in Chemical Sciences	Department of Chemistry, NIT, Trichy, India	9-11 July 2014.
39.	Modelling of Functional Materials From abinitio Calculation	Symposium on Atomic and Molecular Modelling	University of Oslo, Norway	12 June 2014
40.	Multiferroic oxides: Design from first principles calculations	Institute Colloquium	Institute of Mathematical Sciences, Chennai, India	July 3, 2013
41.	Modelling of Multiferroic Oxides	Institute Lecture at Department of Physics	IIT, Kanpur, India	1 November 2013
42.	Advances in Solar Thermal Technologies	Institute Colloquium	IIT, Kanpur, India	2 November 2013
43.	Design of Hydrogen Storage Materials from Abinitio Calculation	Institute Colloquium	Central University of Tamil Nadu, Thiruvarur, India	30 December 2013
44.	Gave series of lectures on Advances in Solar Energy Applications; Solar Irradians and Thermal Collectors, Concentrator Solar Thermal Collector	Refreshers course in Physics	Bharathiyar University, Coimbatore, India	18 September 2013
45.	Effect of Pressure and Nanophase aspects on Hydrogen Storage Materials	International Conference on Materials for Energy and Nano Convergence (ICMENC2013)	Hindustan University, Chennai, India	4-6, July 2013
46.	Chaired an half day oral presentation section	International Conference on Materials for Energy and Nano Convergence (ICMENC2013)	Hindustan University, Chennai, India	4 July 2013

47.	Design of Hydrogen Storage Materials from Abinitio Modelling	First national conference on Mapping the "Materials Genome"	Shiv Nadar University, Noida, Delhi, India	March 8-10, 2013.
48.	Invited lecturer (gave 6 hrs lecture) on recent advances in DFT applications	DFT school in Plasma 2012	Pondicherry University, Pondicherry, India	December 10-12 (2012).
49.	Computational studies on functional materials and energy storage materials	International Conference on Research in Condensed Matter Physics (ICCMP2012)	University of Madras, India	1-3 October 2012
50.	Chaired the first scientific session	International Workshop and Conference on Renewable Energy and Climate Change – Exploring Opportunities for Sustainable Development – IWCRECC-2012	Madurai Kamaraj University, Madurai, India	April 5-7, 2012
51.	Electricity and Magnetism with focus on Computational Physics	Department of Physics	Department of Physics, Norwegian University of Science and Technology (NTNU), Trondheim, Norway	12 Oct. 2011
52.	Atomic and Nanoscale investigation of hydrides	Institute Colloquium	Institute of Mathematical Sciences, Chennai, India	26 September 2011
53.	Modelling of Energy Storage Materials and their Nanophase aspects	Departmental Seminar	Madurai Kamaraj University, Madurai, India	25 July 2011
54.	Nanoscale Modelling of Hydrogen Storage Materials	Institute Colloquium	Central University of Thiruvapur, Tamil Nadu, India	12 August 2011
55.	Atomic and Nanoscale modelling of Materials for Energy Technology	Institute Seminar	SSN Reserch Center, Chennai, India	9 August 2010
56.	Modelling of Materials with Multifunctionality	Institute Colloquium	Max-Planck-Institut fuer Festkoerperforschung, Stuttgart, Germany	22 November, 2010
57.	Nanoscale modelling from <i>ab initio</i> calculations	International Workshop using RSPT code	Uppsala University, Uppsala, Sweden	October 3-8, 2010
58.	Design and Development of Advanced Materials for EEE technologies'	Chief Guest presentation at the inauguration of Materials Research Association	PSG Tech, Coimbatore, India	August 2, (2010)
59.	Abinitio studies on Advanced materials for Energy Technology	Center Colloquium	Center for Study of Science, Technology and	July 30, (2010)

			Policy, Bangalore, India	
60.	Modelling of Advanced Materials and their properties using Density Functional Calculations	Institute Seminar	Department of Materials Engineering, IISc, Bangalore, India	July 26 (2010)
61.	Design and Development of Multifunctional oxides from computational Modelling	Center Seminar	CCMT, IISc, Bangalore, India	July 28 (2010).
62.	Modelling of Hydrogen storage materials – Metal Hydrides & Complex Hydrides	Departmental Seminar	Department of Physics, IISc, Bangalore, India	July 29 (2010)
63.	Modelling of Metal Hydrides and Complex Hydrides	Institute Colloquium	IISER, Trivandrum, India	July 16 (2010)
64.	Simulation of multifunctional Materials based on magnetic materials and transparent conductors	Indo-Swedish conference on Functional materials	Uppsala University, Uppsala, Sweden	June 28-30 (2010)
65.	Modelling of defects and defect complexes in ZnO	Mini-symposium	Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden	June 10 (2010).
66.	Modelling of Solar-energy materials	Institute Seminar	Department of Materials Science, NTNU, Trondheim, Norway	23 March 2010
67.	Hydrogen storage materials – Metal Hydrides and Complex Hydrides	the Psi-k summer school on Computational Nanoscience for Renewable Energy Solutions (CONARES)	Helsinki, Finland	September 14-17 (2009)
68.	Hydrogen storage materials – High pressure and Nanophase aspects	Psi-k summer school on Computational Nanoscience for Renewable Energy Solutions (CONARES)	Helsinki, Finland	September 14-17 (2009)
69.	Modeling of Multifunctional oxides	International Conference on Materials for Advanced Technology, (ICMAT2009)	Singapore	28 June – 3 July (2009)
70.	Modeling of multifunctional oxides and hydrogen storage materials	Institute Colloquium	Institute of Physics and Technology, University of Bergen, Norway	February 6 (2009).
71.	Application of DFT calculations for XPS spectra analysis	XPS workshop	SMN, University of Oslo, Norway	11-12 November (2008).

72.	Giant magnetoelectric effect from density functional calculations	International Workshop on Computational Magnetism and Spintronics (CCMS08)	MPI-PKS, Dresden, Germany	November 03-07 (2008)
73.	Computational Studies of Materials for Hydrogen Storage and a possible new Application of Hydrides	Nordic Network Meeting	Reykjavik, Iceland	June 29-30 (2008)
74.	Density functional calculations for multiferroics, oxygen vacancy ordered $\text{Sr}_4\text{Fe}_4\text{O}_{11}$, and spin-chain compound $\text{Ca}_3\text{Co}_2\text{O}_6$	Institute Seminar	JNCASR, Bangalore, India	12 March (2008)
75.	Multifunctional oxides and hydrogen storage materials from density functional calculation	Institute Seminar	IISER, Pune, India	11 March (2008)
76.	Multifunctional materials from density functional calculations	International conference on Materials Science Research and Nanotechnology, ICMSRN2008	Mother Teresa University, Kodaikanal, India	February 27-29, (2008)
77.	Electronic structure, spin, and valence features of spin-chain compound $\text{Ca}_3\text{Co}_2\text{O}_6$	Institute Colloquium	Laboratoire CRISMAT, Caen, France	25-27, October (2007)
78.	Modeling of multiferroic oxides for sensors	SMN-Wadahl meeting	Wadahl, Norway	21-22 November (2007).
79.	Ab-initio studies on hydrogen storage materials	Institute Seminar	at Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan	16 November (2007).
80.	Origin of magnetoelectric behaviour in BiFeO_3	Nanomaterials conference 2007	Bergan, Norway	4-9 June. (2007)
81.	Theoretical modeling of Multiferroics	Ferroic Functional Elements group seminar	Prof. Lukas Eng at Institut für Angewandte Photophysik, Dresden, Germany	30 May 2007
82.	Spin-, charge-, and orbital-ordering in transition metal oxides	Mini symposium	Royal Institute of Technology, Stockholm, Sweden	29 March 2007
83.	Modeling of magnetoelectric materials	FPLMTO meeting on development of new code	Uppsala University, Uppsala, Sweden	28 August – 01 September 2006
84.	Electronic structure and Optical properties of ZnO , ZnSiO_3 , and Zn_2SiO_4 with point defects	Functional oxides for energy technology (FOET) meeting	NTNU, Trondheim, Norway	2 October, 2006

85.	<i>Theoretical investigation on MgH₂:Ti</i>	Nordic Energy Research Meeting	Soria-Moria, Oslo, Norway	23-24 November 2005
86.	<i>Modeling of hydrogen storage materials using density functional calculations</i>	3 rd International Conference on Materials for Advanced Technologies (ICMAT 2005)	Singapore	3-8 July 2005
87.	<i>Magnesium-based hydrides for hydrogen storage applications</i>	Nordic Energy Research Meeting	Krusenberg, Sweden	17-18 June 2005
88.	<i>Magnetic and ferroelectric properties of BiFeO₃</i>	Spin, Charge, Orbital Ordering in Transition Metal Oxides (SCOOTMO) Meeting	University of Oslo, Oslo, Norway	7-9 May 2005
89.	<i>Magnetism in transition metal oxides</i>	Swedish Summer School on Magnetism and Transport in Solids	Uppsala University, Sweden	14-18 June 2004
90.	Theoretical modelling of hydrogen storage materials	FUNMAT meeting	Olavsgaard, Norway	5-7 January 2005
91.	Spin, Charge, and Orbital ordering in Manganites	FUNMAT meeting	Olavsgaard, Norway	5-7 January 2005
92.	Origin of ferroelectricity in multiferroic BiFeO ₃	FUNMAT meeting	Olavsgaard, Norway	5-7 January 2005
93.	Structural stability of alkali boron hydrides, MBH ₄	FUNMAT meeting	Olavsgaard, Norway	5-7 January 2005
94.	<i>Density-functional studies on mixed-valent chromium oxide</i>	SCOOTMO meeting	AGH University of Science and Technology, Krakow, Poland	24-28 September (2004)
95.	<i>Density functional calculations on functional materials</i>	Seminar on Present and Future research activities in Norway on Functional Materials (FUNMAT)	Gardermoen, Oslo, Norway	27-28 October June (2003)
96.	<i>Magnetic phase diagram studies in Ruthenates</i>	Perovskite Oxide Meeting	Gardermoen, Oslo, Norway	4-5 June (2002).
97.	<i>Excited state properties of perovskite-type oxides from first principle calculations</i>	Perovskite meeting - Autumn 2000	Sundvollen, Norway	Nov. 27-28 (2000).
98.	Applications of Density functional theory	Institute seminar	Institute of Mathematical Sciences, Madras, India	06 November 1998
99.	Calculation of magnetic anisotropy energy from ab-initio methods	Institute seminar	Department of Nuclear Physics, University of Madras, India	30 October 1998
100	Correlation between electronic structure and disorder effects in solids	National Conference on Defects in Condensed Media	Indira Gandhi Center for Atomic Res. Kalpakkam, India	Sep.20-22, 1995

Talks/Presentations in the International Level conferences, meetings, seminars and workshops

S.No	Title	Name of Event	Place of The Event	Date and Year
1.	Magnetic and Magneto-caloric properties of MnBi and Mn (0.94) Cr (0.06) Bi	International school and conference on Evolution of Electronic Structure Theory and Experimental Realization (EESTER 2023, 3rd Edition)	IIT- Madras SRM IST- KTR	January 4 - 12, 2023
2.	The Computational Investigation of an Anticarcinogenic Agent β - elemene using Density Functional Theory	International school and conference on Evolution of Electronic Structure Theory and Experimental Realization (EESTER 2023, 3rd Edition)	IIT- Madras SRM IST- KTR	January 4 - 12, 2023
3.	First principles investigations on the charge carrier transport properties of Rb ₂ SnBr ₆	International Conference on Nanotechnology: Opportunities and Challenges, 2022 (ICNOC-2022)	Jamia Millia Islamia, New Delhi, India	November 28-30, 2022
4.	Two Dimensional Si ₂ BNO ₄ : A Potential Material for Optoelectronic Applications- an <i>Ab- Initio</i> Study	International Conference on Nanotechnology: Opportunities and Challenges, 2022 (ICNOC-2022)	Jamia Millia Islamia, New Delhi, India	November 28-30, 2022
5.	Computational analysis of novel Heusler alloys for spin polarized and thermoelectric device applications	International Union of Materials Research Society, International Conference in Asia – 2022 (IUMRS-ICA 2022).	Indian Institute of Technology Jodhpur, India	19-23 December 2022
6.	First Principles Study on the Structural, Electronic, and Optical Properties of Mixed Cation-Mixed halide Vacancy-ordered Double Perovskite Compound KRbSnBr ₃ I ₃ ,	6 th International Conference on Nanoscience and Nanotechnology (ICONN-2021)	SRM University, Chennai, India	February 01 – 03, 2021
7.	Revealing the optoelectronic properties of tin-based vacancy ordered double perovskites: K ₂ SnBr ₆ and Rb ₂ SnBr ₆	National Conference on Physics and Chemistry of Materials (NCPCM-2020)	Govt. Holkar Science College, Indore, India	14th- -16th December, 2020
8.	First principles prediction of the ground state crystal structures of antiperovskite compounds A ₃ PN (A= Be, Mg, Ca, Sr, Ba and Zn).	International Conference on Materials for Energy and Environment (ICMEE-2018)	Loyola Institute of Frontier Energy, Chennai, India	February 22 & 23, 2018
9.	Design of Magnetoelectric Multiferroics	International conference on electronic structure	Stuttgart, Germany	12-15, June 2013

		methods held at Max Planck Institute		
10.	Modelling of defects and defect complexes in semiconductors	International conference on electronic structure methods held at Max Planck Institute	Stuttgart, Germany	12-15, June 2013
11.	Theoretical studies on borohydrides	NANOMAT-H meeting	SINTEF, Oslo, Norway	23 June (2010)
12.	Modeling of Hydrogen storage Materials	Nordic Energy Meeting	Svalbard, Norway	April 19-22, 2010
13.	Modeling of mixed alanates	NANOMAT-H meeting	Institute of Energy Technology, Kjeller, Norway	22 March 2010
14.	Role of transition metal substitution in complex hydrides – theory	NANOMAT-H meeting	NTNU, Trondheim, Norway	15 December 2009
15.	<i>Ab initio studies of optical properties of ZnX (X=O, S, Se, Te).</i>	E-MRS meeting,	Nice, France	May29 to June 2, 2006
16.	<i>Ab initio studies of electronic structure and optical properties of zinc silicates ZnSiO₃ and dizinc orthosilicates Zn₂SiO₄</i>	E-MRS meeting	Nice, France	May29 to June 2, 2006
17.	<i>Electronic structure and optical properties of indium tin oxide.</i>	1st international symposium on transparent conducting oxides	Hersonissos, Crete, Greece	23 – 25 October 2006
18.	<i>Chemical-bonding and High-pressure Studies on Hydrogen-storage Materials</i>	International Conference on Materials for Advanced Technologies (ICMAT 2003)	MRS, Singapore	7-12 December 2003
19.	<i>Elastic properties and phonons in borocarbides</i>	International conference of electronic structure theory in honor of the 60'th birthday of Prof. B. Johansson	Uppsala University, Uppsala, Sweden	10-11 June (2002).
20.	<i>Electronic structure and magnetic properties of LaXO₃ (X=Sc-Cu) from full-potential calculation</i>	Ψ_{k2000} Conference, <i>Ab initio (from electronic structure) calculation of complex process in Materials,</i>	Schwäbisch Gmünd, Germany	Aug.22-26, 2000
21.	<i>Anomalous orbital magnetism: VAu₄</i>	Ψ_{k2000} Conference, <i>Ab initio (from electronic structure) calculation of</i>	Schwäbisch Gmünd, Germany	Aug.22-26, 2000

		<i>complex process in Materials</i>		
22.	<i>Electronic structure studies on superconducting MgB₂ and related compounds</i>	8th European Conference on Solid State Chemistry	Oslo, Norway	4-7 July (2001).
23.	<i>First-principle calculations for electronic structure and magneto-optical properties of AuMnSn and AuMnSb</i>	8th European Conference on Solid State Chemistry	Oslo, Norway	4-7 July (2001).
24.	<i>Spin, Charge, and Orbital ordering and electronic bandstructure studies on reduced perovskites YBaMn₂O₅ and Ca₃Co₂O₆</i>	8th European Conference on Solid State Chemistry	Oslo, Norway	4-7 July (2001).
25.	<i>Theoretical Investigation of Hydrides Based on CuAl₂-type Materials</i>	8th European Conference on Solid State Chemistry	Oslo, Norway	4-7 July (2001).
26.	<i>IR and Raman active phonons and spin-state transition from WIEN97</i>	Fifth WIEN workshop on Full-Potential LAPW calculations with the WIEN97 code	Vienna University of Technology, Vienna, Austria	April 7-10 1999
27.	<i>Calculation of Single Crystal Elastic Constants for Structural Intermetallics from First Principles</i>	5th IUMRS International Conf. in Asia	Bangalore, India	Oct.13-16, (1998)
28.	<i>High Pressure Studies and the Role of Interstitials on Elastic and Cleavage Properties of Ti₃Al</i>	5th IUMRS International Conf. in Asia	Bangalore, India	Oct.13-16, (1998)
29.	<i>Magnetic Anisotropy, Magnetic, Optical and Magneto-Optical Properties of Selected Binary Intermetallics</i>	5th IUMRS International Conf. in Asia	Bangalore, India	Oct.13-16, (1998)
30.	<i>Magnetic, Optical and Magneto-Optical properties of Cerium and Uranium monochalcogenides</i>	28 ^{emes} Journées des Actinides	Uppsala, Sweden	May. 14-16 (1998)
31.	<i>Giant magneto-crystalline anisotropy and magneto-optical effects in binary intermetallics</i>	Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces	Technische Universität Wien, Austria	June 3-7 (1998)
32.	<i>Calculated magneto-optical spectra of 3d elements and compounds</i>	Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces	Technische Universität Wien, Austria	June 3-7 (1998)

33.	<i>Pressure induced hexagonal to cubic structural transition in Ti_3Al from WIEN95 comparison with TBLMTO and FLMTO results</i>	HCM-WORKSHOP, Full-Potential LAPW calculations with the new WIEN97 code	Vienna University of Technology, Austria	July 1-5, 1997
34.	<i>Electronic structure, phase stability and high pressure studies on superconducting and non-superconducting rear-earth transition metal borocarbides</i>	Psi-k Network Conference, <i>Ab initio (from electronic structure) calculation of complex process in Materials</i>	Schwäbisch Gmünd, Germany	Sept.17-21, 1996
35.	<i>Stability and electronic structure of metastable gold silicide Au_7Si</i>	Psi-k Network Conference, <i>Ab initio (from electronic structure) calculation of complex process in Materials</i>	Schwäbisch Gmünd, Germany	Sept.17-21, 1996
36.	<i>Phase stability studies of Ti_3X ($X=Al, Ga$ or In) and $Ni_3(Al, Nb)$ systems from electronic structure calculations</i>	International conference on Physical Metallurgy, ICPM-94	BARC, Bombay, India	November 1994
37.	<i>Electronic band structure of some of the Laves phase and structural intermetallic compounds</i>	International workshop on Electronic Structure Calculations and Properties of Materials	Anna University, Madras, India	Nov.16-21, 1992
38.	<i>Electronic structure and superconductivity of YX ($X=S, Se$ or Te)</i>	International workshop on Electronic Structure Calculations and Properties of Materials	Anna University, Madras, India	Nov.16-21, 1992
39.	<i>Pressure induced metallisation in some of the alkali iodides</i>	International workshop on Electronic Structure Calculations and Properties of Materials	Anna University, Madras, India	Nov.16-21, 1992

Talks/Presentation in the National Level conferences, meetings, seminars and workshops

S.No	Title	Name of Event	Place of The Event	Date and Year
1.	Presentation of Strategic Vision Plan to Build Centralized Computation, Synthesis & Characterization Facilities, create an interdisciplinary Computational Modeling center, creation of Department of Material Science and Nanotechnology as well as Department of Energy and Environmental Science	Academic Council Meeting of CUTN	Qutub Hotel, Delhi	21 April 2012

2.	Build a center on "Chemistry and Physics of Energy Materials and Nanostructures	Discussion meeting	Rica Hotel, Oslo, Norway	7-8 April (2011)
3.	Chairman for a few sessions	Meeting on recent developments in SMN	Wadah, Norway	27-29 November 2006
4.	<i>Electronic structure, Phase stability and equation of state studies on structural and superconducting intermetallics</i>	DAE Solid State Physics Symposium'95	IACS, Jadavpur, Calcutta, India	Dec.27-31, 1995
5.	<i>Electronic structure and Equation of State studies on superconducting and non-superconducting rare-earth transition metal borocarbides</i>	2 nd National Conference on High Pressure Science and Technology	Guru Ghasidas Univ., Bilaspur, India	Nov.9-11, 1995
6.	<i>Pressure induced B1 to B2 structural transition and EOS Studies on superconducting Lanthanum mono chalcogenides</i>	2 nd National Conference on High Pressure Science and Technology	Guru Ghasidas Univ., Bilaspur, India	Nov.9-11, 1995
7.	<i>Pressure induced hexagonal to cubic phase transition in high temperature ordered structural intermetallics</i>	2 nd National Conference on High Pressure Science and Technology	Guru Ghasidas Univ., Bilaspur, India	Nov.9-11, 1995
8.	<i>"Pressure induced metallisation in some of the alkali iodides</i>	2 nd National Conference on High Pressure Science and Technology	Guru Ghasidas Univ., Bilaspur, India	Nov.9-11, 1995
9.	<i>Structural phase transition and metallisation induced by pressure in CaF₂</i>	2 nd National Conference on High Pressure Science and Technology	Guru Ghasidas Univ., Bilaspur, India	Nov.9-11, 1995
10.	<i>Structural stability of Zr₃Al from electronic structure studies</i>	Solid State Physics Symposium	Bhabha Atomic Research Center, Bombay, India	Dec.27-31, 1993
11.	<i>Equation of states and Ground State properties of YGa₂ and LaGa₂</i>	Solid State Physics Symposium	Bhabha Atomic Research Center, Bombay, India	Dec.27-31, 1993
12.	<i>s,p to d electron transfer and pressure induced superconductivity in elemental Bismuth</i>	Solid State Physics Symposium	Sri Venkateswara University, Tirupathi, India	Dec. 28 1992- Jan 1, 1993
13.	<i>Pressure induced metallisation in BaX (X=O,S,Se or Te)</i>	Solid State Physics Symposium	Sri Venkateswara University, Tirupathi, India	Dec. 28 1992- Jan 1, 1993

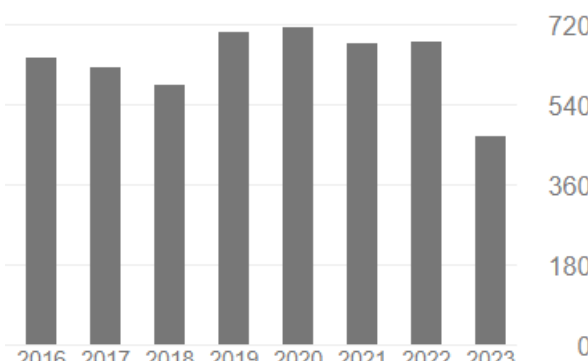
Participation without talks in the International/National Level conferences, meetings, seminars and workshops

S.No	Name of Event	Place of The Event	Date and Year
1.	15 th JNC conference on Chemistry of Materials	"Vivanta by Taj" Kovalam, Thiruvananthapuram, Kerala.	Sept 30, 2019 - Oct. 2, 2019
2.	Two days lecture workshop on Recent Developments in Chemistry	Department of Chemistry, Central University of Tamil Nadu, India	2-3, March (2016).

3.	15 th European Seminar on Computational Methods in Quantum Chemistry - 2011(ESCMQC'11)	Oscarsborg, Norway	16-19 June (2011)
4.	NANOMAT-H meeting	SINTEF, Oslo, Norway	31 August (2010)
5.	Nordic Energy Meeting, NTNU	Trondheim, Norway	15 Dec. (2009)
6.	International symposium on Metal-Hydrogen systems (MH2008)	Reykjavik, Iceland	June 24-28 (2008).
7.	Summer School on "Materials for the Hydrogen Society"	Reykjavik, Iceland	June 19-23 (2008)
8.	International conference on Nano spintronics Design and Realization (ICNDR 2007)	Max-Planck Institute, Dresden, Germany	21-25 May (2007)
9.	Summer School on 'Materials for the hydrogen economy.	University of Iceland, Reykjavik, Iceland	26-30 June 2006
10.	Nanotechnology consortium Spring 2006 meeting	Cambridge, UK	1-2 June 2006
11.	2 nd International Symposium on Hydrogen in Matter (ISOHIM),	Uppsala, Sweden	13-17 June 2005
12.	Workshop on <i>ab initio</i> phonon calculations	Polish Academy of Sciences, Krakow, Poland,	1-4 December (2004)
13.	Workshop on "Abinitio Modelling of Solid State Chemistry (MSSC2003)	University of Torino, Italy	7-12 September(2003).
14.	Workshop on "Correlation Effects in Electronic Structure Calculations	ICTP, Trieste, Italy	17-21 (2002)
15.	Symposium on the <i>Quantum Mechanical Basis For Materials Properties</i>	Hjortviken, Sweden	Feb.19-Feb.21 1998
16.	28 th Journees des Actinides	Uppsala, Sweden	May 14-16 (1998)
17.	The Graduate School Programme in Materials Science <i>Electronic structure of solid Materials</i>	Royal Institute of Technology, Materialfysik, KTH, Stockholm, Sweden	Aug.21-30 1997
18.	International Workshop on Electronic structure calculations and properties of Materials	Anna University, Madras, India	Nov.16-21, 1992
19.	XIII AIRAPT International Conference on High Pressure Science and Technology	National Aeronautical Laboratory, Bangalore, India	Oct.7-11, 1991
20.	Group Discussion meeting on New Insights into the Old Hubbard Model	Institute of Mathematical Sciences, Madras, India	Feb.25-March 1, 1991
21.	Workshop on Electronic Structure of Random Alloys	S.N. Bose National Center for Basic Sciences, Calcutta, India	Nov.20-Dec.5, 1990

22.	National Symposium on Band structure and its applications to the study of properties of Materials	Anna University, Madras, India	Feb.13-15, 1990
23.	Solid State Physics Symposium	Indian Institute of Technology, Madras, India	1. Dec. 28-31, 1989.

LIST OF PUBLICATIONS:

	National	International	Google Scholar Citations as on 03.07.2023	
Number of papers published (In Number)	8	188	All	Since 2018
Number of Books Published (In Number)	2 (Edited)	4 Book Chapters	Citations	10182
			h-index	49
			i10-index	118
				

Books Edited:

1. Crystal growth and Computational Materials Science, Macmillan Publishers India Ltd, (2012) ISBN:978-935-059-048-5
2. Energy and Eco-Friendly Materials, Macmillan Publishers India Ltd, (2011) ISBN:978-935-059-047-8

Book Chapters:

1. P.Ravindran, G.Subramoniam, and R.Asokamani, Phase stability studies of Ti₃X (X=Al,Ga,In) and Ni₃ (Al,Nb) systems from electronic structure calculations, in Advances in Physical Metallurgy, CRC press ISBN:9782884492102 p.407-410 (2023).
2. P.Vajeeston, P. Ravindran, and H. Fjellvåg, Chemical bonding in Hydrides, in Advances in Chemical Research, Editor James C.Taylor, Nova Sci. Pub. Inc. ISBN 978-1-61324-018-2, Vol.10, Ch.5 p.1-24 (2011).

3. U. Grossner, S. Zh. Karazhanov, and P.Ravindran *Computational materials science. Fundamentals and application to ZnO and GaN*, Wide Band Gap Materials and New Developments, Editors: Mikael Syvajarvi and Rositza Yakimova ISBN: 81-308-0092-6 (2006).
4. R.Asokamani, P.Ravindran, and G. Pari, *Crystal structure transitions in aerospace materials and magnetic phase transitions in inorganic cubic perovskites at high pressures*, in Advances in High Pressure Science and Technology, Ed. by A.K.Singh, Tata McGraw-Hill, New Delhi, p.35-47, (1995).

A. Review Articles:

1. P.Vajeeston, P.Ravindran and H. Fjellvåg, *Predicting new materials for hydrogen storage application*, **Invited review** for the special issue on "Energy Technology for the 21st Century - Materials and Devices", Materials **2**, 2296-2318, (2009).
2. V.A. Yartys, P. Vajeeston, A.B.Riabov, P.Ravindran, R.V.Denys, J.P.Maehlen, R.G.Delaplane, and H.Fjellvåg *Crystal chemistry and metal-hydrogen bonding in anisotropic and interstitial hydrides of intermetallics of rare earth (R) and transition metals (T), RT_3 and R_2T_7* , Z. Kristallogr. **223**, 674–689, (2008).
3. P. Ravindran, R. Vidya, P. Vajeeston, A.Kjekshus and H. Fjellvåg *Ground state and excited state properties of inorganic solids from full-potential density functional calculations* J. Solid State Chemistry (**Invited review**) **176** , 338-374 (2003).

B. Published articles in international refereed journals:

2023:

1. Mukesh K Choudhary, Helmer Fjellvåg, P Ravindran, First principle studies on electronic and thermoelectric properties of Fe_2TiSn based multinary Heusler alloys, Computational Materials Science **216**, 111856, (2023)
2. Vishnu Sudarsanan, Anu Maria Augustine and P Ravindran, $Na_2Mn(CO_3)_2$: A carbonate based prototype cathode material for Na-ion batteries with high rate capability-An ab-initio study, Electrochimica Acta **439**, 141687 (2023)
3. Kiruthika S, Sundar P and P Ravindran, Structural phase stability and thermodynamical properties of transition metal complex hydrides Na_2MgTMH_7 (TM= Sc to Cu) for hydrogen storage applications, Journal of Solid State Chemistry **321**, 123867 (2023).
4. G. Kruthika and P. Ravindran, Discerning the crystal structure and engineering the optoelectronic properties through substitution of divalent cations (M= Zn, N = Ge) in $C_3H_3M_xN_{1-x}I_3$ for solar cell applications, Mater. Sci. in Semicond. Processing **160**, 107449 (2023)
5. S Kiruthika and P. Ravindran, First principle study on transition metal ammine borohydrides with amphoteric hydrogen for hydrogen storage applications, International Journal of Hydrogen Energy (2023).
6. AM Augustine, V Sudarsanan, P Ravindran, Suppressing the initial capacity fade in Li-rich Li_5FeO_4 with anionic redox by partial Co substitution—a first-principles study, Sustainable Energy & Fuels **7** (6), 1502-1521 (2023)
7. T. Santy and P. Ravindran, Two Dimensional Si_2BNO_4 : A Potential Material For Optoelectronic Applications - An *Ab-Initio* Study, Springer Proceedings in Materials in press (2023).
8. PD Sreedevi and P Ravindran, First principles investigations on the charge carrier transport properties of Rb_2SnBr_6 , Springer Proceedings in Materials in press (2023).

2022:

9. Mukesh K Choudhary, P Ravindran, First principle design of new thermoelectrics from TiNiSn based pentanary alloys based on 18 valence electron rule, Computational Materials Science, 209, 111396, (2022)
10. PD Sreedevi, R Vidya and P Ravindran, Antiperovskite materials as promising candidates for efficient tandem photovoltaics: First-principles investigation, Materials Science in Semiconductor Processing, 147 ,(2022).
11. D. Shobana Priyanka, J. B. Sudharsan, M. Srinivasan, P. Ramasamy, Mukesh K. Choudhary, and P. Ravindran, First-principles calculations to investigate new ferromagnetic quaternary Heusler alloys FeZrTiZ (Z=Si, Sn, Pb): compatible for spin polarized device and waste heat recovery applications, Solid State Sciences (2022)
12. G Kruthika and P Ravindran, Understanding the optoelectronic properties of interface between Cs₂TiBr₆ and TiO₂ for solar cell applications, Materials Today Communications (2022)
13. A. Krishnamoorthy and P. Ravindran, X-ray Magnetic Circular Dichroism Spectra for Uranium Mono-Chalcogenides, UQ (Q=S, Se, and Te) from First Principles, J. of Physical Chem. C 126(46) 19792-19802 (2022)
14. PD Sreedevi, and P Ravindran, Elucidating the Photovoltaic effect of Monoclinic K₂SnBr₆ by Mixed-Cation Mixed-Halide Substitution from First-Principles Calculations, J. Phys. D:App. Phys, 56(3) 035104 (2022).

2021

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