

Curriculum vitae

Dr. G. S. Vaitheeswaran

Assistant Professor

Advanced Centre of Research in High Energy Materials (ACRHEM)

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Objective

A strong dedication towards scientific research and interest in teaching Physics and Chemistry.

Personal details

Name : Ganapathy Subramanian Vaitheeswaran
Father's Name : Ganapathy Subramanian
Nationality : Indian
Sex : Male
Date of Birth : 24-07-1975
Marital status : Married
Present Designation : Assistant Professor, Advanced Centre of Research in High Energy Materials (ACRHEM), University of Hyderabad

Educational Qualifications

Ph.D (Theoretical Condensed Matter Physics) obtained from Anna University during 1999-2004.

M.Sc (Physics) pursued from Annamalai University during 1995-1997.

B.Sc (Physics) obtained from University of Madras during 1992-1995.

Research Interests

- Study of energetic materials under high pressures using first principles calculations
- Investigating equation of state of crystalline solids
- Predicting physical and chemical properties of solids through *ab-initio* calculations
- Magnetism in solids
- Evolution of band structure of complex materials

Research Experience

- **Guest Scientist** in Max-Planck institute for solid state Research, Stuttgart, Germany from March 2003 to July 2005
- **Researcher** in Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm, Sweden from August 2005 to Aug 2007.
- **Visiting Scientist** in Advanced Centre of Research in High Energy Materials (ACRHEM), University of Hyderabad from 24th September 2007 to 5th June 2009

Research Publications as on 15th May 2013

NUMBER OF CITATIONS (as on 15th May 2013): 667

h-index: 16

(ISI WEB OF KNOWLEDGE)

(These figures represent number of times my papers were cited in different research articles)

68. K. Ramesh Babu, **G. Vaitheeswaran**, 2013, "Lattice dynamics and electronic structure of energetic solids: A first principles study" Chem. Phys. Lett. In press. (IF:2.145)
67. V. Kanchana, N. Yedukondalu, **G. Vaitheeswaran**, 2013, "Structural, elastic, electronic, and optical properties of layered alkaline-earth halofluoride scintillators " Phil. Mag. 93, 26, 3563.
66. K. Ramesh Babu, **G. Vaitheeswaran**, 2013, "Structural, elastic and thermodynamic properties of KN₃ and RbN₃: A van der Waals density functional study" Solid State Sciences, 23, 17. (IF:1.856)
65. J. Ramanna, N. Yedukondalu, K. Ramesh Babu, **G. Vaitheeswaran**, 2013, "Ab initio study of electronic structure, elastic and optical properties of anti-perovskite type alkali metaloxyhalides" Solid State Sciences, 20, 120. (IF:1.856)
64. S. Appalakondaiah, **G. Vaitheeswaran**, S. Lebègue, 2013, "A DFT study of structural, elastic, vibrational and quasi particle band structure of solid nitro methane" Journal of Chemical Physics, 138, 184705. (IF: 3.3)
63. N. Yedukondalu, Vikas D Ghule and **G. Vaitheeswaran**, 2013, "Pressure induced structural phase transition in solid oxidizer KClO₃: Ab initio study" Journal of

Chemical Physics, 138, 174701. (IF: 3.3)

62. R. S. Kumar, A. Svane, **G. Vaitheeswaran**, Y. Zhang, V. Kanchana, M. Hofmann, S. J. Campbell, Y. Xiao, P. Chow, C. Chen, Y. Zhao, A. L. Cornelius, 2013, "Pressure-Induced valence and structural changes in YbMn_2Ge_2 Inelastic X-ray spectroscopy and Theoretical investigation" *Inorg. Chem*, 52 (2), 832. (IF: 4.6)
61. U. Subba Rao, A. Sebastian, S. Rayaprol, C. S. Yadav, A. Svane, **G. Vaitheeswaran**, and S. C. Peter, 2013, "Metal flux crystal growth technique in the determination of ordered superstructure in EuInGe " *Crystal Growth & Design*, 13 (1), 352. (IF: 4.72)
60. S. Appalakondaiah and **G. Vaitheeswaran**, 2013, "Structural properties of solid nitromethane: A Density functional study" *AIP Conference Proceedings*, 1512, 830.
59. S. Yagoubi, S. Heathman, A. Svane, **G. Vaitheeswaran**, P. Heines, J. C. Griveau, T. LeBihan, M. Idri, F. Wastin, R. Caciuffo, 2013, "High pressure studies on Uranium and thorium silicide compounds: Experiment and theory", *J. Alloys. Compds*, 546, 63. (IF: 2.289)
58. **G. Vaitheeswaran** and K Ramesh Babu, 2012, "Metal azides under pressure: an emerging class of high energy density materials", *J. Chemical Sciences*. 124, 1391. (IF: 1.17)
57. Ch. Bheema Lingam, K. Ramesh Babu, Surya P Tewari and **G. Vaitheeswaran**, 2012, "High pressur study of structural and vibrational properties of ammonia borane" *J. Phys. Conf. Series* 377, 012088
56. N. Yedukondalu, **G. Vaitheeswaran**, 2012, "Vibrational properties of BaClF , BaBrF and BaIF under pressure" *J. Phys. Conf. Series*, 377, 012070.
55. S. Appalakondaiah, **G. Vaitheeswaran**, S. Lebegue, N. E. Christensen, A. Svane, 2012, "Effect of vanderWaals interactions on structural and elastic properties of black phosphorus" *Phys. Rev. B*, 86, 035105. (IF: 3.691)
54. N. Yedukondalu, Vikas D Ghule and **G. Vaitheeswaran**, 2012, "Computational study of structural, electronic and optical properties of crystalline NH_4N_3 " *J. Phys. Chem. C*. 116, 16910. (IF: 4.8)
53. Swetarekha Ram, V. Kanchana, **G. Vaitheeswaran**, A. Svane, S. B. Dugdale, and N. E. Christensen, 2012, "Electronic topological transition in LaSn_3 under pressure" *Phys. Rev. B*. 85, 174531. (IF: 3.691)
52. J. Staun Olsen, J.-E. Jørgensen, L. Gerward, **G. Vaitheeswaran**, V. Kanchana, A. Svane, 2012, "Compressibility and structural stability of CeN from experiment and theory: The B1-B2 transition" *J. Alloys and Compds*. 533, 29. (IF: 2.289)

51. K. Ramesh Babu, **G. Vaitheeswaran**, 2012, "Ab initio study of structural and vibrational properties of KN_3 under pressure" *Chem. Phys. Lett.* 533, 35. (IF: 2.337)
50. **G. Vaitheeswaran**, V. Kanchana, X. Zhang, Yanming Ma, A. Svane, S. N. Kaul, 2012, "Lattice instability and martensitic transformation in LaAg predicted from first-principles theory" *J. Phys.: Cond. Matt.* 24, 075402. IF (2.546)
49. Ch. Bheema Lingam, K. Ramesh Babu, Surya P Tewari and **G. Vaitheeswaran**, 2012, "Density functional study of Electronic, Bonding, and Vibrational Properties of $\text{Ca}(\text{NH}_2\text{BH}_3)_2$ " *J. Comp. Chem.* 33, 987. (IF: 4.05)
48. V. Kanchana, **G. Vaitheeswaran**, Xinxin Zhang, Yanming Ma, A. Svane, and O. Eriksson, 2011, "Lattice dynamics and elastic properties of the 4f electron system: CeN" *Phys Rev B* 84, 205135. (IF: 3.691)
47. Ch. Bheema Lingam, K. Ramesh Babu, Surya P Tewari and **G. Vaitheeswaran**, 2011, "Electronic structure and optical properties of $\text{Ca}(\text{NH}_2\text{BH}_3)_2$ studied from GW calculations" *J. Phys Chem C*, 115, 18795. (IF: 4.8)
46. A. Waškowska, L. Gerward, J. Staun Olsen, K. Ramesh Babu, **G. Vaitheeswaran**, V. Kanchana, A. Svane, V.B. Filipov, G. Levchenko and A. Lyaschenko, 2011, "Thermo-elastic properties of ScB_2 , TiB_2 , YB_4 and HoB_4 : Experimental and Theoretical studies", *Acta Materialia*, 59, 4886-4894 (IF: 3.781)
45. **G. Vaitheeswaran**, V. Kanchana, A. Svane, N. Christensen, J. Staun Olsen, J. E. Jorgensen, L. Gerward, 2011, "High-pressure structural study of yttrium monochalcogenides from experiment and theory", *Phys. Rev. B*, 83, 184108 (IF: 3691)
44. K. Ramesh Babu, Ch. Bheema Lingam, Surya P Tewari, **G. Vaitheeswaran**, 2011, High-pressure study on Lithium azide from density functional calculations, *J. Phys. Chem A*, 115, 4521. (IF: 2.946)
43. N. Yedu kondalu, K. Ramesh Babu, Ch. Bheema Lingam, D.J. Singh, **G. Vaitheeswaran**, V. Kanchana, 2011, "Electronic structure, optical and bonding properties of alkaline-earth halofluoride scintillators BaClF , BaBrF , BaIF ", *Phys. Rev. B*, 83, 165117 (IF: 3.691)
42. Ch. Bheema Lingam, K. Ramesh Babu, Surya P Tewari, **G. Vaitheeswaran**, 2011, Structural, electronic, bonding and elastic properties of NH_3BH_3 : A Density functional study, *J. Comp. Chem.*, 32, 1734. (IF: 4.05)

41. J. Staun Olsen, A. Waskowska, L. Gerward, **G. Vaitheeswaran**, V. Kanchana, A. Svane, N. Shitsevalova and V. B. Filipov, 2011, HoB₄ at high pressure and low temperature: An experimental and theoretical study, *High Pressure Research* 31, No:1, 3-6. (IF: 0.7)
40. K. Ramesh Babu, Ch. Bheema Lingam, S. Auluck, Surya P Tewari, **G. Vaitheeswaran**, 2011, Structural, thermodynamic and optical properties of MgF₂ studied from first principles theory, *J. Solid State Chem* 184, 343. (IF: 2.159)
39. Ch. Bheema Lingam, K. Ramesh Babu, Surya P Tewari, **G. Vaitheeswaran**, 2011, Quantum chemical studies on BeH₂ oligomers *Computational and Theoretical Chem* 963, 371. (IF: 1.228)
38. Ch. Bheema Lingam, K. Ramesh Babu, Surya P Tewari, **G. Vaitheeswaran** and S. Lebègue, 2011, Quasi particle band structure and optical properties of NH₃BH₃ *Phys. Status Solid RRL* 5, No:1, 10. (IF: 2.815)
37. V. Kanchana, **G. Vaitheeswaran**, P. Souvatzis, O. Eriksson, S. Lebègue, 2010, "Density functional study of electronic structure and lattice dynamics of SrCl₂", *J. Phys.: Cond. Matt*, 22, 445402. (IF: 2.5)
36. **G. Vaitheeswaran**, V. Kanchana, Ravhi kumar S, A. L. Cornelius, M. F. Nicol, A. Svane, N. E. Christensen, O. Eriksson, 2010, "High pressure structural study of fluoro-perovskite CsCdF₃ up to 60 GPa : A combined experimental and theoretical study", *Phys. Rev B* 81 075105 (IF: 3.691)
35. V. Kanchana, **G. Vaitheeswaran**, Yanming Ma, Yu Xie, A. Svane, and O. Eriksson, 2009, "Density functional study of elastic and vibrational properties of the Heusler-type alloys Fe₂VAl and Fe₂VGa", *Phys. Rev. B*, 80, 125108. (IF: 3.691)
34. A Winkler, N Narayanan, D Mikhailova, K G Bramnik, H Ehrenberg, H Fuess, **G. Vaitheeswaran**, V Kanchana, F Wilhelm, A Rogalev, A Kolchinskaya and L Alff, 2009, "Magnetism in Re-based ferimagnetic double perovskites", *New J Physics*, 11, 073047.
33. Staun Olsen, L. Gerward, **G. Vaitheeswaran**, V. Kanchana, and L. Alff, 2009, "High-pressure structural behavior of the double perovskite Sr₂CrReO₆: An experimental and theoretical study", *High Pressure Research*, 29, 83-86 (2009). (IF: 0.7)
32. **G. Vaitheeswaran**, V. Kanchana, M. Alouani and A. Delin, 2008, "Ab initio calculated X-ray magnetic circular dichroism of Sr₂CrReO₆", *Euro Physics Letters* 84, 47005. (IF: 2.171)
31. Ravhi S. Kumar, A. L. Cornelius, A. Svane, **G. Vaitheeswaran**, V. Kanchana, Eric D.

- Bauer, M. Hu and M. F. Nicol, 2008, "Pressure-induced valence change in YbAl_3 : A combined high pressure inelastic x-ray scattering and theoretical investigation", *Phys. Rev. B* 78, 075117. (IF: 3.691)
30. V. Kanchana, **G. Vaitheeswaran**, and A. Svane, 2008, "Calculated structural, elastic and electronic properties of SrCl_2 ", *Journal of Alloys and Compounds*, 455, 480. (IF: 2.289)
29. F. S. Yel'kin, V. A. Sidorov, A. Was'kowska, L. Gerward, J. Staun Olsen, **G. Vaitheeswaran** and V. Kanchana, 2008, "Phase transitions in Cd_3P_2 at high pressures and high temperatures", *J. Alloys and Compounds*, 450, 79. (IF: 2.289)
28. V. Kanchana, **G. Vaitheeswaran**, M. Alouani, A. Delin, 2007, "Electronic structure and x-ray magnetic circular dichroism of $\text{Sr}_2\text{FeMoO}_6$: Ab initio calculations", *Phys. Rev. B (Rapid Communications)*, 75, 220404. (IF: 3.691)
27. Y. Krockenberger, K. Mogare, M. Reehuis, M. Tovar, M. Jansen, **G. Vaitheeswaran**, V. Kanchana, F. Bultmark, A. Delin, F. Wilhelm, A. Rogalev, A. Winkler, and L. Alff, 2007, " $\text{Sr}_2\text{CrOsO}_6$: End point of a spin-polarized metal-insulator transition by 5d band filling", *Phys. Rev. B (Rapid Communications)* 75, 020404. (IF: 3.691)
26. **G. Vaitheeswaran**, V. Kanchana, S. Heathman, M. Idiri, T. Le Bihan, A. Svane A. Delin, and B. Johansson, 2007, "Elastic constants and high-pressure structural transitions in lanthanum monochalcogenides from experiment and theory", *Phys. Rev. B*, 75, 184108. (IF: 3.691)
25. **G. Vaitheeswaran**, V. Kanchana, R. S. Kumar, A. L. Cornelius, M. F. Nicol, A. Svane, A. Delin and B. Johansson, 2007, "High-pressure structural, elastic and electronic properties of the scintillator host material, KMgF_3 ", *Phys. Rev. B*, 76, 014107. (IF: 3.691)
24. **G. Vaitheeswaran**, V. Kanchana, A. Svane, A. Delin, 2007, "Elastic properties of MgCNi_3 – a superconducting perovskite", *Journal of Physics Condensed Matter*, 19, 326214. (IF: 2.5)
23. V. Kanchana, **G. Vaitheeswaran**, A. Svane and A. Delin, 2006, "First-principles study of elastic properties of CeO_2 , ThO_2 and PoO_2 ", *Journal of Physics: Condensed Matter*, 18, 9615. (IF: 2.5)
22. V. Kanchana, **G. Vaitheeswaran**, and M. Alouani, 2006, "Calculated electronic structure and x-ray magnetic circular dichroism of CrO_2 ", *Journal of Physics: Condensed Matter*, 18, 5155. (IF: 2.5)
21. **G. Vaitheeswaran**, V. Kanchana and A. Delin, 2006, "Electronic structure of the ferromagnetic double-perovskites $\text{Sr}_2\text{CrReO}_6$, Sr_2CrWO_6 , B_2FeReO_6 ", *Journal of Physics: Conference series*, 29, 50-53.

20. P. Majewski, S. Geprägs, A. Boger, M. Opel, A. Erb, R. Gross, **G. Vaitheeswaran**, V. Kanchana, A. Delin, F. Wilhelm, A. Rogalev and L. Alff, 2005, “Magnetic moments of W 5d in Ca_2CrWO_6 and Sr_2CrWO_6 double perovskites”, *Phys. Rev.B*, 72,32402. (IF: 3.691)
19. L.Gerward, J. Staun Olsen, L. Petit, **G.Vaitheeswaran**, V. Kanchana, A. Svane, 2005, “Bulk modulus of CeO_2 and PrO_2 – An experimental and theoretical study”, *Journal of Alloys and Compounds*, 400, 56-61. (IF: 2.289)
18. **G.Vaitheeswaran**, V. Kanchana and Anna Delin, 2005, “Pseudo-half-metallicity in the double perovskite $\text{Sr}_2\text{CrReO}_6$ from density functional calculations”, *Applied Physics Letters*, 86, 032513. Article selected for the January 24, 2005 issue of *Virtual Journal of Nanoscale Science and Technology* (IF: 3.84)
17. A. Svane, V. Kanchana, **G.Vaitheeswaran**, G. Santi, W.M. Temmerman, Z.Szotek, P.Strange and L.Petit, 2005, “Electronic structure of Samarium monopnictides and monochalcogenides”, *Physical Review B*, 71, 045119. (IF: 3.691)
16. **G.Vaitheeswaran**, L. Petit, A. Svane, V. Kanchana and M. Rajagopalan, 2004, “Electronic structure of Praseodymium monopnictides and monochalcogenides under pressure”, *Journal of Physics Condensed Matter*, 16, 4429. (IF: 2.5)
15. J. Staun Olsen, L. Gerward, V. Kanchana and **G.Vaitheeswaran**, 2004, “The bulk modulus of ThO_2 - an experimental and theoretical study”, *Journal of Alloys and Compounds*, 381, 37. (IF: 2.289)
14. A. Svane, G. Santi, Z. Szotek, W. M.Temmerman, P. Strange, M. Horne, **G.Vaitheeswaran**, V. Kanchana , L. Petit and H.Winter, 2004, “Electronic structure of Sm and Eu Chalcogenides”, *phys. stat. soli.(b)*, 241, 3185. (IF: 1.316)
13. **G.Vaitheeswaran**, V.Kanchana and M.Rajagopalan, 2003, “Theoretical studies on the high pressure phases of Lanthanum monochalcogenides”, *Journal of Physics and Chemistry of Solids*, 64, 15. (IF: 1.632)
12. V.Kanchana, **G.Vaitheeswaran** and M.Rajagopalan, 2003, “Pressure induced structural phase transitions and metallization of BaF_2 ”, *Journal of Alloys and Compounds*, 359, 66. (IF: 2.289)
11. V.Kanchana, **G.Vaitheeswaran** and M.Rajagopalan, 2003, “High-pressure structural phase transitions in magnesium fluoride studied by electronic structure calculations”, *Journal of Alloys and Compounds*, 352, 60. (IF: 2.289)
10. V. Kanchana, **G.Vaitheeswaran** and M. Rajagopalan, 2003, “Electronic structure of Ionic PbFCl -type compounds under pressure”, *Journal of Physics: Condensed Matter*, 15, 1677. (IF: 2.5)
9. V. Kanchana, **G.Vaitheeswaran** and M. Rajagopalan, 2003, “Structural phase stability of

- CaF₂ and SrF₂ under pressure”, *Physica B*, 328, 283. (IF: 1.063)
8. **G.Vaitheeswaran**, V.Kanchana and M.Rajagopalan, 2002, “Structural phase stability and superconductivity of LaN”, *Solid State Communications*, 124, 97. (IF: 1.649)
 7. **G.Vaitheeswaran**, V. Kanchana and M. Rajagopalan, 2002, “Electronic and Structural properties of LaSb and LaBi”, *Physica B*, 315, 64. (IF: 1.063)
 6. **G.Vaitheeswaran**, V. Kanchana and M. Rajagopalan, 2002, “Theoretical study of LaP and LaAs at high pressures”, *Journal of Alloys and Compounds*, 336, 46. (IF: 2.289)
 5. P. Selvamani, **G.Vaitheeswaran**, V. Kanchana and M. Rajagopalan, 2002, “Effect of pressure on the superconducting transition temperature of Nb-Zr and Ti-V”, *Physica C*, 370, 108. (IF: 1.01)
 4. V.Kanchana, **G.Vaitheeswaran**, and M.Rajagopalan, 2002, “Pressure-induced structural and magnetic phase transition in ferromagnetic CrTe”, *Journal of Magnetism and Magnetic Materials*, 250, 353. (IF: 1.780)
 3. M. Rajagopalan, P. Selvamani, **G.Vaitheeswaran**, V. Kanchana and M. Sundareswari, 2001, “Calculation of superconducting transition temperature of MgB₂” *Solid State Communications*, 120, 215. (IF: 1.649)
 2. **G.Vaitheeswaran**, I. B. Shameen Banu and M. Rajagopalan, 2000, “Theoretical calculation of superconducting transition temperature in Vanadium under pressure” *Solid State Communications*, 116, 401. (IF: 1.649)
 1. I.B. Shameen Banu, M. Rajagopalan and **G.Vaitheeswaran**, 2000, “Structural and Bonding properties of Intermetallic compounds ARh₂P₂(A=Ca, Sr, Ba)” *Solid State Communications*, 116, 451. (IF: 1.649)

Honours and Awards

- ▶▶ Elected as **Member of National Academy of Sciences India** (Physical Sciences) - 2013.
- ▶▶ Recipient of “**DAE-Young Achiever**” Award for the year 2012 from **Department of Atomic Energy**.
- ▶▶ Honored with **Associate Fellow of Andhra Pradesh Academy of Sciences (AFAPASc)** for valuable contributions towards the scientific research in condensed matter physics.

- ▶▶ Recipient of Max-Planck Institute Post Doctoral Fellowship for the duration of March 2003- July 2005.
- ▶▶ Recipient of Swedish Research Council Post Doctoral Fellowship for the duration of August 2005- August 2007.
- ▶▶ Received **KAWZOE AWARD** for **“best paper presentation”** in “Third conference on Asian Consortium on Computational Material Science” held during 8th September to 11th September 2005 at Chinese Academy of Sciences, Beijing, China.
- ▶▶ Received **KAWZOE AWARD** for **“best paper presentation”** in “First conference on Asian Consortium on Computational Material Science” held during 29th November to 1st December 2001 at Indian Institute of Science, Bangalore, India.

Invited talks

- ★ An invited talk on **“Solid energetic materials: A First principles study”** has been given at Work shop on Advances in computational physics 2013 held at Central University of Tamilnadu, February-2013, Thiruvarur, Tamilnadu, India.
- ★ An invited talk on **“High energy density materials: A First Principles Study”** has been given at Electronic structure approaches to atoms, molecules, solids and clusters, January-2013, ACRHEM, University of Hyderabad, India.
- ★ An invited talk on **“High Pressure study of energetic metal azides: A First principles study”** has been given at DAE-Solid State Physics Symposium 2012 held at IIT Bombay, December-2012, India.
- ★ An invited talk on **“High pressure study of inorganic metal azides”** has been given at NCL-Pune, November-2012, India.
- ★ An invited talk on **““Lattice instability and structural transformation in LaAg predicted from first principles theory”** has been given at Indian Institute of Technology Kharagpur, November-2012, India.
- ★ An invited talk on **“Azides: An emerging class of high energy density materials”** has been given at Frontiers in Physics, FIP-2012, University of Hyderabad, September-2012, India.
- ★ An invited talk on **“Lattice instability and structural transformation in LaAg under pressure: A first principles study”** has been given at NCMAT-2012, IIIT-Gwalior, Gwalior, February-2012, India.

- ★ Delivered an invited talk on “**Metal azides under pressure: an emerging class of high energy materials**” in MTIC-2011, University of Hyderabad, Hyderabad, December-2011.
- ★ An invited talk on “**Alkali metal azides under high pressure: *Ab-initio* study**” has been delivered at AIRAPT-2011, BARC Mumbai, Mumbai, India.
- ★ An invited talk presented on “**Exploring material properties from abinitio calculations**” at Inter University Accelerator Center (IUAC), New Delhi, April 2010.
- ★ A talk on “**Understanding the high-pressure behavior of materials from first-principles theory**” delivered upon an invitation in Theoretical Physics Division, Bhabha Atomic Research Center, Mumbai, March 2009.
- ★ A talk on “**Effect of Spin orbit coupling on the band gaps of half-metallic double perovskites**” delivered upon an invitation in Solid State Physics Division, Bhabha Atomic Research Center, Mumbai, March 2010.
- ★ A talk on “**Metal-Insulator transition induced by 5d-band filling ferromagnetic double perovskites**” delivered upon an invitation at National Physical Laboratory (NPL), New Delhi, October 2008.
- ★ A talk entitled “**Elastic properties of MgCNi₃: A super conducting perovskite**” delivered at work shop on Low Temperature Physics, University of Hyderabad, Hyderabad, March 2008.
- ★ A talk on “**Understanding magnetism in double perovskites from first-principles studies**” delivered at Advanced Centre of Research in High Energy Materials (ACRHEM), University of Hyderabad, Hyderabad, April 2007.
- ★ An invited seminar delivered on “**High-pressure structural studies on binary rare-earth antimonides**” at Denmark Technical University, Copenhagen during August 2006.
- ★ An invited seminar on “**Orbital magnetism in double perovskites**” delivered at Walther-Meissner-Institute, Garching, Germany in June 2006.
- ★ A talk presented upon an invitation at the Institute for Materials Science, Darmstadt University of Technology, Darmstadt, Germany on “**First principles study of electronic structure and magnetic properties of double perovskites**” during June 2005.
- ★ An invited seminar delivered on “**Electronic structure and magnetic properties of transition metal oxides**” at the Walther-Meissner- Institute, Garching, Germany during April 2005.

Contributed talks

- ★ A talk on “**Nitrogen rich high energy density materials:A density functional study** ” has been given at KISHEM-2012, Inha University, September-2012, South Korea.
- ★ Delivered contributed talk on “**Cubic to orthorhombic transition in binary inter metallic Compound LaAg predicted from first-principles theory**” at ICMST-2012, International Conference on Materials Science and Technology, ICMST-2012 held at St. Thomas College, Pala, Kerala, India
- ★ Delivered contributed talk on “**Density functional study of hydrogen rich solid rocket propellants metal amido boranes**” at HEMCE-2011, International conference on High Energy Materials, HEMCE-2011 held at TBRL-Chandigarh, India.
- ★ Delivered contributed presentation on “**Density functional study of LiN₃ and KN₃ molecular crystals under pressure**” at ACCMS-6, Sptember 2011, National University of Singapore, Singapore.
- ★ A talk entitled “**Equation of state of high density fluoro perovskite KMgF₃ studied from first principles theory**” delivered at Indo-Russian work shop on High Energy Density Materials, I²IT, Pune, November 2008.
- ★ Delivered a contributed talk on “**Electronic Structure and X-ray circular dichroism of half-metallic transition metal oxides**” at International Conference on Magnetic Materials and their Applications fo 21st Cemtury (MMA-21), National Physical Laboratory (NPL), New Delhi, October 2008.
- ★ Delivered a talk on “**Unquenched orbital magnetic moments in Rhenium based double perovskites**” at International Conference on Magnetic Materials, Saha Institute of Nuclear Physics, December 2007.

Posters presented in Conferences

1. Presented a poster paper entitled “**Structural properties of solid nitromethane: A Density functional study**” S. Appalakondaiah and **G. Vaitheeswaran** during DAE- Solid State Physics Symposium 2012, held at IIT- Bombay, during December-2012, India
2. Presented a poster paper entitled “**Lattice dynamics of alkali metal azides studied from density functional perturbation theory**” **G. Vaitheeswaran** during the **ICORS-2012**, held at Indian Institute of Science, Bangalore.
3. Presented a poster paper entitled “**Density functional study of high capacity hydrogen storage materials: metal amidoboranes**” Ch. Bheema Lingam, K. Ramesh Babu, S.P. Tewari, and **G. Vaitheeswaran** during the Modern Trends in Inorganic Chemistry MTIC-2011, held at University of Hyderabad, Hyderabad.

4. Presented a poster paper entitled “**Computational study of structural, elastic constants and related mechanical properties and their relevance to decomposition of alkali metal azides**” K. Ramesh Babu, Ch. Bheema Lingam, **G. Vaitheeswaran** and S.P. Tewari, proceedings of HEMCE-2011, International conference on High Energy Materials, HEMCE-2011 held at TBRL-Chandigarh, India.
5. Presented a poster paper entitled “**Pressure induced phase transitions in RbBH₄**” K. Ramesh Babu, Ch. Bheema Lingam, S.P. Tewari, and **G. Vaitheeswaran** during the International conference on High Pressure Science (AIRAPT-2011) held at Bhabha Atomic Research Centre (BARC, Mumbai) on 25 to 30 September 2011.
6. Presented a poster paper entitled “**Structural and vibrational properties of NH₃BH₃ under high pressure**” Ch. Bheema Lingam, K. Ramesh Babu, S.P. Tewari, and **G. Vaitheeswaran** during the International conference on High Pressure Science (AIRAPT-2011) held at Bhabha Atomic Research Centre (BARC, Mumbai) on 25 to 30 September 2011.
7. Presented a poster paper entitled “**Temperature and density effects on solid Nitromethane**” S. Appalakondaiah, Moumita Saharay, S.P. Tewari, and **G. Vaitheeswaran** during the International conference on High Pressure Science (AIRAPT-2011) held at Bhabha Atomic Research Centre (BARC, Mumbai) on 25 to 30 September 2011.
8. Presented a poster paper on “**Vibrational properties of BaFCl, BaFBr, BaFI under pressure**” N. Yedukondalu, **G. Vaitheeswaran** during the International conference on High Pressure Science (AIRAPT-2011) held at Bhabha Atomic Research Centre (BARC, Mumbai) on 25 to 30 September 2011.
9. Presented a poster paper entitled “**Electronic structure, vibrational and thermodynamic properties of alkali metal azides**” K. Ramesh Babu, Ch. Bheema Lingam, Surya P. Tewari, and **G. Vaitheeswaran** during the International conference on Recent trends in Materials Science and Technology (ICMST-2011) held at Indian Institute of Space Science and Technology IIST, Thiruvananthapuram, Kerala on 29 to 31 October 2010. This paper got **Best Poster Presentation** award.
10. Presented a poster paper entitled “**Electronic structure of NH₃BH₃ oligomers**” Ch. Bheema Lingam, K. Ramesh Babu, S.P. Tewari, and **G. Vaitheeswaran** during the International conference on Recent trends in Materials Science and Technology (ICMST-2011) held at Indian Institute of Space Science and Technology IIST, Thiruvananthapuram, Kerala on 29 to 31 October 2010.

11. Presented a poster paper entitled “**Ab-initio study of Electronic, structural, bonding and elastic properties of NH_3BH_3** ” Ch. Bheema Lingam, K. Ramesh Babu, **G. Vaitheeswaran** and S.P. Tewari during International work shop on Frontiers in Electronic structure calculations: Techniques and Applications on 15th to 17th February 2010 at Department of Physics, University of Pune, Pune, India. Same also presented during Indo-Singapore Joint Physics Symposium 2010 at University of Hyderabad, Hyderabad, India.
12. Presented a poster paper entitled “**Ab-initio study of Electronic structure and bonding properties of LiAlH_4** ” K. Ramesh Babu, Ch. Bheema Lingam, **G. Vaitheeswaran** and S.P. Tewari during International work shop on Frontiers in Electronic structure calculations: Techniques and Applications on 15th to 17th February 2010 at Department of Physics, University of Pune, Pune, India. Same also presented during Indo-Singapore Joint Physics Symposium 2010 at University of Hyderabad, Hyderabad, India.
13. Presented a poster paper entitled “**Structural, electronic, elastic and thermodynamic properties of MgF_2** ” K. Ramesh Babu, Ch. Bheema Lingam, **G. Vaitheeswaran** and S.P. Tewari, 179, proceedings of HEMCE-2009 in International conference on High Energy Materials, HEMCE-2009, at HEMRL - Pune, India.
14. Presented a poster paper entitled “**Electronic and Optical properties of MgH_2** ” Ch. Bheema Lingam, K. Ramesh Babu, **G. Vaitheeswaran** and S.P. Tewari, 179, proceedings of HEMCE-2009 in International conference on High Energy Materials, HEMCE-2009, at HEMRL - Pune, India.
15. Presented a poster paper entitled “**Spectral studies on one dimensional $(\text{BeH}_2)_n$ oligomers**” Ch. Bheema Lingam, **G. Vaitheeswaran** and S.P. Tewari during DAE-BRNS National symposium on Atomic, Molecular and Optical Physics at IUAC- New Delhi on 10th to 13th February 2009, New Delhi, India.
16. Presented a poster paper entitled “**Ab-initio calculations of BeH_2 crystal and BeH_2 polymer**” Ch. Bheema Lingam, S.P. Tewari and **G. Vaitheeswaran** during International Conference on Hydrogen and Hydrogen storage methods and materials at IISc Bangalore on 3rd to 6th January 2009, Bangalore, India.
17. Presented a poster paper entitled “**Effect of band filling on the electronic structure of double perovskites**” **G. Vaitheeswaran**, V. Kanchana, A. Delin, M. Alouani, L. Alff, during the 3rd Indo-Japan conference on Ferroics and Multi Ferroics at IACS Kolkata on 4th to 6th Feb 2008.

18. A poster entitled “**CaNiH₃: A brittle metallic perovskite hydride**” G. Vaitheeswaran at the International Conference on Hydrogen and Hydrogen storage methods and materials at IISc Bangalore on 3rd to 6th January 2009, Bangalore, India.
19. Attended ICMS-ICMR winter school on **New Carbon Materials and Functional Oxides** during 08th December 2008 to 13th December 2008 at JNCASR, Bangalore.
20. Attended Trends in **Computational Materials Science** organized by the Center for Computational Materials Science (CCMS), Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR) during February 15-17, 2007 at JNCASR, Bangalore, India.

Academic Visits

- ✦ Visited Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm, Sweden, during June 2004 and April 2005 for collaborative project on double Perovskite.

- ✦ Visited Institute of Physics and Chemistry of Materials, University of Strassbourg, (CNRS) France, during December 2003, for working on the optical properties of CrO₂

- ✦ Visited Department of Physics, University of Aarhus, Aarhus, Denmark, during November 2003, August 2006 and July 2007 for a combined project on ‘*f*’ electrons and double perovskites.

- ✦ Visited Department of Physics, University of Aarhus, Aarhus, Denmark, during August 2002, for a part of my Ph.D work (SIC-LSD studies on Pr pnictides and Chalcogenides).

Declaration

I (**G.S. Vaitheeswaran**) hereby declare that the above said information is correct to the best of my knowledge and supervision.

Yours faithfully