Curriculum Vitae of Professor S. Ramasesha

**1.** Name : S. Ramasesha

**2.** Date of Birth : January 16, 1950

**3.** Present Position : Emeritus Professor and INSA Honorary Scientist

**4.** Permanent Address: Solid State and Structural Chemistry Unit

Indian Institute of Science Bangalore 560 012, INDIA

1. Education: B.Sc. (Hons.) (I Rank) from Central College, Bengaluru and M.Sc. (I Rank) and Ph.D. from IIT Kanpur
2. Post-doctoral work: University of Oxford, England, UK, Princeton University, NJ, USA
3. Employment: Joined as Assistant Professor in IISc., Bengaluru in 1984
4. Current Position: Emeritus Professor and INSA Honorary Scientist, SSCU, IISc., Bangalore
5. Visiting Professor Positions: Visiting Professor at Princeton University, USA; University of Arizona USA, Institute for Nanostructured Materials, Bologna, CNR Italy, University of Mons, Belgium, University of Bordeaux, France, Ecole Normale Superiere, Cachan, France, International Institute of Physics, Natal, Brazil.
6. Distinctions:

(i) National Science Talent Scholar, 1965-1973

(ii) General Proficiency Award, Indian Institute of Technolgy, Kanpur 1970

(iii) Indian National Science Academy medal for young scientists', 1978

(iv) B.M. Birla National Science Prize in Chemistry, 1990

(v) Honorary Fellow: 1991-1998. Honorary Professor: 1998 – Jawaharlal Nehru Centre for

Advanced Scientific Research

(vi) Elected Fellow of the Indian Academy of Science, 1992.

(vii) Awarded the Shanti Swarup Bhatnagar Prize of the Council of Scientific and

Industrial Research, India, 1992.

(viii) Honorary Faculty, S.N. Bose National Centre for Basic Sciences 1994-1997.

(ix) Amrut Mody Professor of Chemical Sciences, 2000-2003

(x) Elected Fellow of the Indian National Science Academy, 2005.

(xi) Awarded the J. C. Bose National Fellowship, 2006 - 2016.

(xii) Awarded silver medal of the Chemical Research Society of India, 2008.

(xiii) Awarded the IISc Alumni Award for Excellence in Research, 2008.

(xiv) Elected Fellow of The World Academy of Sciences for the Developing World (TWAS), 2011.

(xv) Awarded Sir M. Visvesvaraya senior scientist award by the Government of Karnataka for lifetime achievement, 2018.

(xvi) Conferred Honorary Fellowship of the Karnataka Science and Technology Academy.

**Citation Summary:** Total Citations: 7258, H-Index 45, I10-index 125 (Google Scholar, May 03, 2022)

1. **Highlights of Ramasesha’s research contributions**

(Reference numbers correspond to papers in list of publications)

* The puzzle of Polytypism in solids was solved by showing that polytypes arise from the Lifshitz’s phases of the Anisotropic Next Nearest Neighbour Ising (ANNNI) model. (202, 218)
* Introduced bit representation of valence bond (VB) diagrams and bit manipulations for exact diagonalization of large interacting systems, in collaboration with Professor Soos. (207)
* Extended the VB method for obtaining exact dynamic response of strongly correlated systems by a correction vector (CV) approach, in collaboration with Professor Soos. (187,194)
* Introduced a small matrix algorithm for solving large sparse system of linear algebraic equations, arising in the context of CV approach. (178)
* Developed a bilinear basis technique to solve the long standing problem of exploiting spin and spatial symmetries of systems belonging to nonAbelian point groups. (39,67)
* Developed a VB method for spin coupling arbitrary spins in a molecular magnetic cluster. (228)
* Developed real time dynamics of wave packets within the VB approach. (90,108)
* Developed a perturbative approach to compute magnetic anisotropy of single molecule magnets. (66)
* Introduced symmetrized density matrix renormalization group (DMRG) technique to obtain desired excited states of strongly correlated systems. (138)
* Introduced CV technique for dynamic response of strongly correlated systems in the DMRG approach. (125)
* Introduced symmetry adapted quantum Monte Carlo method for excited states of Hubbard models. (119)
* Showed electron correlations destroy the solitonic midgap state and obtained model exact excited states of polyenes. (204,205)
* Showed the origin of fluorescence in some organic polymers. (156)
* Solved the puzzle of singlet-triplet branching ratios in the electron-hole recombination process in conjugated systems. (90,108)
* Obtained quantum phase diagrams of dimerized and frustrated spin chains in collaboration with Professor Diptiman Sen. (145)
* Explained the switch over from ferromagnetic to antiferromagnetic exchange in Rare Earch-Cu ion systems. (96)
* Using DMRG method, studied finite temperature properties of alternating spin chains. (120, 121, 124)
* Obtained excited states and magnetization dynamics of several single molecule magnets. (101-104)
* Using modified real time DMRG method, studied spin-charge separation in polyenes. (34, 37, 43)
* Studied Peierls’ instability and excited state crossover in polyacenes by the DMRG method. (98, 99)
* Theoretically demonstrated frustration as a paradigm for obtaining bulk magnetization in conjugated carbon systems. (30, 14)
* Combining exact diagonalization method and kinetic Monte Carlo method, obtained Blocking Temperature of Single Chain Magnets and showed why single rare earth ion magnets have large Blocking Temperature. (1)

1. **List of PhD Theses Guided**
2. “Diagrammatic Valence Bond Theory: Application to One-Dimensional Kondo Lattice Model and

Extension to Ab Initio Molecular Calculations” - Krishna Das, 1989.

1. “A Theoretical Study of the Linear and Non-linear Optical Properties of Conjugated Systems” -I. D. L.

Albert, 1991.

1. “Theoretical Studies on Models for Organic Ferromagnetism” - Bhabadyuti Sinha, 1993.
2. “Monte Carlo Simulations of Condensed Phases of Hydrocarbons and Studies of the Correlated

Electronic Structure of Large Conjugated Systems” - Aparna Chakrabarti, 1995.

1. “Quantum Monte Carlo and Configuration Interaction Studies of the Ground and Excited States

of the Hubbard Model: Application to Fullerenes and Other Large Correlated Systems” – Bhargavi Srinivasan, 1996.

1. “Properties of the Correlated Electronic States in Conjugated Organic Molecules, Polymers and

Metal-Halogen Chains” - Y. Anusooya, 1996.

1. “Density Matrix Renormalization Group Studies of Low- Dimensional Magnetic Systems and

Conjugated Polymers” - Swapan Kumar Pati, 1998.

1. “Theoretical Studies of (i) Electronic States and Electron - Hole Recombination in -Conjugated

Systems and (ii) Magnetic properties of Spin Ladders” - Kunj Tandon, 2000.

1. “Theoretical Studies of Electronic and Magnetic Properties of Molecular and Extended Low-

Dimensional Materials” - Raghu C, 2001.

1. “Theoretical Studies of Single Molecule Magnets and Frustrated Spin Lattices” - Indranil

Rudra, 2004.

1. “Theoretical Studies of Electronic and Optical Properties of Some Heteroconjugated Systems”

- Prakash Chandra Jha, 2005.

12. “Theoretical Studies on Electronic Properties of Conjugated Systems: Low Lying Excitations and Dynamics of Electron - Hole Recombination, Triplet – Triplet Scattering and Singlet” -Mousumi Das, 2006.

13. “Theoretical approaches for modeling molecular magnetism” - R Rajamani, 2008.

14 “Theoretical Studies of the Electronic States in Conjugated Molecules and Quantum Phase Diagrams of Interacting One-Dimensional Models” - Manoranjan Kumar, 2008.

15. “Theoretical Studies of Electronic Properties and Electronic Processes in Conjugated Molecules” – Sukrit Mukhopadhyay, 2010.

16. “Real Time DMRG Dynamics of Spin and Charge Transport in Low-Dimensional Strongly CorrelatedSystems” – Tirthankar Dutta, 2011.

17. “Modelling Electronic Properties of Strongly Correlated Conjugated Molecular Systems” – SimilThomas, 2012.

18. “Studies of Electronic, Magnetic and Entanglement Properties of Correlated models in Low-Dimensional Systems” – Shaon Sahoo, 2012.

19. “Studies on Frustrated Spin Chains and Quasi-One-Dimensional Conjugated Carbon Systems” –V.M.L. Durgaprasad Goli, 2014.

20. “Theoretical Investigations of Opto-Electronic Processes in Organic Conjugated Systems within IInteracting Models: Exact Diagonalization and DMRG Studies” – Suryoday Prodhan, 2017

21. “Theoretical Studies of Skewed Spin Ladders and Polycyclic Aromatic Hydrocarbons“ – Geetanjali Giri, 2019

22. “Modeling Magnetic Anisotropy in Single Chain Magnets” – Sumit Haldar, 2020

23. “Quantum Phases and Magnetization Plateaus of Skewed Spin Ladders” – Sambunath Das (2021)

**12.List of Master’s Theses Guided**

1. Ms. Bhargavi Srinivasan
2. Mr. Saifi Khan
3. Mr. Indranil Rudra
4. Mr. Srinivasan Varadharajan
5. Ms. N. Jayashree
6. Mr. Tirthankar Dutta
7. Mr. Sukrit Mukhopadhyay
8. Mr. Shaon Sahoo
9. Mr. Oinam Nganba
10. Mr. Agnish Behera (UG)

**13. Courses Taught**

1. Introductory Chemical Physics

2. Physical Chemistry

3. Mathematics for Chemists

4. Computational Chemistry

5. Quantum Mechanics and Group Theory

6. Topics in Solid State Chemistry

7. Principles of the Solid State

8. NPTEL course on “Bonds and Bands in Solids”

9. Coordinated and conducted over twenty Academies as well as JNC workshops on various topics ranging from Quantum Chemistry, Electronic Properties of Molecules for Organic Electronic Devices, Electron States in Low-Dimensional Systems, Molecular Spectroscopy and Nonlinear Optics.

10. Mentored many Indian Academies Summer research Fellows.

11. Hosted about a dozen post-doctoral fellows.

**14. List of Publications**

1. S. Haldar and **S. Ramasesha**, (2021), “[Study of magnetization relaxation in molecular spin](javascript:void(0))

[clusters using an innovative kinetic Monte Carlo method](javascript:void(0))”, Phys. Rev. **B** 103, 214424**.**

1. Sambunath Das, Dayasindhu Dey, Manoranjan Kumar and S. Ramasesha (2021), “Quantum

phases of a frustrated spin-1 system: the 5/7 skewed ladder”, Phys. Rev. B 104, 125138.

1. Sambunath Das, Dayasindhu Dey, **S. Ramasesha** and Manoranjan Kumar, (2021), “Quantum phases of spin-1 system on 3/4 and 3/5 skewed ladders”, J. Appl. Phys. 129 (22), 223902.
2. S. Haldar and **S. Ramasesha**, (2020), “Magnetocaloric Effect in Molecular Spin Clusters: Exact and Monte Carlo Studies Using Exact Cluster Eigen States”, J. Mag. Mag. Mater. **500**, 166424.
3. D. Dey, S. Das, M. Kumar and **S. Ramasesha**, (2020) “[Magnetization plateaus of spin- system on a](javascript:void(0))

[5/7  skewed ladder](javascript:void(0))” Phys. Rev., B **101**, 195110.

1. A. Valentim, G.A. Bocan, J.D. Fuhr, D.J. Garcia, G. Giri. M. Kumar and **S. Ramasesha** (2020), “A

simple scheme for finding magnetic aromatic hydrocarbon molecules”, Phys. Chem. Chem. Phys.,

**22**, 5882.

1. Geetanjali Giri, Y. Anusooya Pati and **S. Ramasesha**, (2019) "The Correlated Electronic States of a

Few Polycyclic Aromatic Hydrocarbons: A Computational Study”, J. Phys. Chem A, **123**, 5257.

1. S. Prodhan, S. Mazumdar and **S. Ramasesha**, (2019) “Correlated Electronic Properties of a

Graphene Nanoflake Coronone”, Molecules, **24,** 730.

1. Geetanjali Giri, Suryoday Prodhan, Y. Anusooya Pati and **S. Ramasesha**, (2018) “A Model Exact Study of the Properties of Low-Lying Electronic States of Perylene and Substituted Perylenes”, J. Phys. Chem., A, **122**, 8650.
2. Sumit Haldar, Rajamani Raghunathan, Jean-Pascal Sutter and **S. Ramasesha**, (2018) “Modeling

Molecular Magnets with Large Exchange and On-Site Anisotropies”, Phys. Rev. B **98**, 214409.

1. S. Prodhan and **S. Ramasesha**, (2018) “Symmetrized density matrix renormalization group algorithm for low-lying excited states of conjugated Carbon systems: Application to 1, 12- Benzopyrene and poly chrysene”, Phys. Rev. B **97**, 195125.
2. Sumit Haldar, Rajamani Raghunathan, Jean-Pascal Sutter and **S. Ramasesha,** (2017) “Modelling magnetic anisotropy of single chain magnets in |d/J| >> 1 regime”, Mol. Phys., **115,** 2849.
3. S. Prodhan and S. **Ramasesha**, (2017) “[Exact wave packet dynamics of singlet fission in unsubstituted and substituted polyene chains within long-range interacting models](javascript:void(0))”, Phys. Rev. B 96 (7), 07514.
4. G. Giri, D. Dey, M. Kumar, **S. Ramasesha**, Z.G. Soos , (2017) “[Quantum phases of frustrated two-leg spin-1/2 ladders with skewed rungs](javascript:void(0))”, Phys. Rev., B 95 (22), 224408.
5. Y. Anusooya and **S. Ramasesha**, (2017) “Tuning low-energy excitons in substituted tetracenes for singlet fission”, Computational and Theoretical Chemistry, 1116, 151.
6. Arun Kumar Bar, NayanmoniGogoi, Céline Pichon, V. M. L. Durga Prasad Goli, **S. Ramasesha**, MehrezTlijeni, Carine Duhayon, Nicolas Suaud, Nathalie Guihery, Anne-Laure Barra, and Jean-Pascal Sutter, (2017) “[Pentagonal Bipyramid FeII Complexes: Robust Ising‐Spin Units towards Heteropolynuclear Nanomagnets](javascript:void(0))”, Chemistry-A European Journal 23 (18), 4380-4396.
7. V.M.L. Durgaprasad Goli, S. Prodhan, S. Mazumdar and **S. Ramasesha** (2016) “Correlated electronic properties of some graphene nano ribbons: A DMRG study”, Phys. Rev. B **94,** 035139.
8. Manoranjan Kumar, Aslam Parvej, Simil Thomas, **S. Ramasesha** and Z.G. Soos, (2016) “Efficient density matrix renormalization group algorithm to study Y junctions with integer and half-integer spin”, Phys Rev B **93** 075107.
9. Arun Kumar Bar, Celine Pichon, NayanmoniGogoi, Carine Duhayon, **S. Ramasesha,** and Jean-Pascal Sutter (2015),”Single ion magnet behaviour of heptacoordinated Fe(II) complexes: on the importance of supramolecular organization”, Chemical Communications, **51**, 3616.
10. S. Prodhan, Z.G. Soos and **S. Ramasesha** (2014) “Model for triplet state engineering in organic light emitting diodes” J. Chem. Phys. **140**, 214313.
11. Anusooya Y. Pati, **S. Ramasesha** (2014) “An Exact Solution of the PPP Model for Correlated Electronic States of Tetracene and Substituted Tetracene” J. Phys. Chem. **A 118**, 4048.
12. Mei Zhu, Peng Hu,Yungai Li, Xiufeng Wang, Licun Li, Daizheng Liao, V M L Durga Prasad Goli, **S. Ramasesha**, Jean-Pascal Sutter (2014) “Novel Hetero-tri-spin [2p-3d-4f] Chains Compounds Based on [Nitronyl Nitroxide-Ln] Metallo-Ligands: Synthesis, Structure and Magnetic Properties”, Chem. Euro. J., **20**, 13356.

1. Mousumi Das and **S. Ramasesha**, (2014) "A model exact study of two-photon absorption intensities in oligomers of thiophene and pyrrole", Nonlinear Optics Quantum Optics , **43**, 213.
2. Shaon Sahoo, V M L Durga Prasad Goli, Diptiman Sen and **S Ramasesha**, (2014), “Studies on a frustrated Heisenberg spin chain with alternating ferromagnetic and antiferromagnetic exchanges”, J. Phys.: Condens. Matter **26**, 276002.
3. K. Paudel, D. Moghe, M. Chandrasekhar, P. Yu, S. Ramasesha, U. Scherf, and S. Guha,(2013)“Pressure dependence of singlet-triplet excitons in amorphous polymer semiconductors”, Euro Phys Letts., **104**, 27008.
4. M. Kumar, **S. Ramasesha** and Z.G. Soos, (2013) “Quantum phase diagram of one-dimensional spin and Hubbard models with transitions to bond order wave phases”, Croatica Chemica Acta, **86**, 407.
5. Simil Thomas, Anusooya Pati and **S. Ramasesha**, (2013) “"Linear and Non-Linear Optical Properties of Expanded Porphyrins: A DMRG Study"”, J. Physical Chem. A **117**, 7804.
6. V. M. L. Durga Prasad Goli, Shaon Sahoo, **S. Ramasesha**, Diptiman Sen, (2013)" Quantum phases of dimerized and frustrated Heisenberg spin chains with s = 1/2, 1 and 3/2: an entanglement entropy and fidelity study", J. Phys. Condens. Matter, **25,** 125603. arXiv:1208.0706
7. Ravindra Pandey, Sukrit Mukhopadhyay, **S. Ramasesha**, P.K. Das and Joseph Zyss, "Influence of anion on the quadratic nonlinearity and depolarization ratios of scattered second harmonic light from cation π-complexes", J. Chem. Phys. **136**, 194504, http://dx.doi.org/10.1063/1.4716020.
8. Simil Thomas, **S. Ramasesha**, Karen Hallberg and Daniel Garcia, (2012) "Fused azulenes: Possible organic Multiferroics", Phys. Rev. B. Rapid Comm, **86**, 180403; DOI:10.1103/PhysRevB. 86.180403.
9. Manoranjan Kumar, **S. Ramasesha** and Zoltan G. Soos (2012), "Density matrix renormalization group algorithm for Bethe lattices with spin 1/2 or 1 sites with Heisenberg antiferromagnetic exchange"**,** Phys. Rev. B **85**, 134415.
10. Shaon Sahoo, Jean-Pascal Sutter and **S. Ramasesha**, (2012) “Study of Low Temperature Magnetic Properties of a Single Chain Magnet With Alternate Isotropic and Non-Collinear Anisotropic Units”, arXiv:1110.0933v1 , J. Stat. Phys. 147, 181; DOI 10.1007/s10955-012-0460-7.
11. Manoranjan Kumar, Y. AnusooyaPati and **S. Ramasesha**, (2012) “A Density Matrix Renormalization Group Method Study of Optical Properties of Porphines and Metalloporphines”, J. Chem. Phys., **136**, 014112.
12. Tirthankar Dutta and **S. Ramasesha**, (2012) "Real-time density matrix renormalization dynamics of spin and charge transport in push-pull polyenes and related systems", Phys. Rev., B **85**, 035122.
13. Shaon Sahoo, V.M.L. Durgaprasad Goli, **S. Ramasesha** and Diptiman Sen, (2012) "Exact entanglement studies of strongly correlated systems: Role of long-range interactions and symmetries of the system", J. Phys. Condens. Matter, **24** 115601 doi:10.1088/0953-8984/24/11/115601.
14. Ravindra Pandey, Sampa Ghosh, Sukrit Mukhopadhyay, **S. Ramasesha** and Puspendu Das, (2011) "Geometry and quadratic nonlinearity of charge transfer complexes in solution using depolarized hyper-Rayleigh scattering", J. Chem. Phys., **134**, 044533.
15. Tirthankar Dutta and **S. Ramasesha**, (2011) "Effect of dimerization on dynamics of spin-charge separation in Pariser-Parr-Pople model: A time dependent density matrix renormalization group study", Phys. Rev. B **84**, 235147.
16. Sukrit Mukhopadhyay, Ravindra Pandey, Puspendu Das and **S. Ramasesha**, (2011) " Geometry and quadratic nonlinearity of charge transfer complexes in solution: A theoretical study", J. Chem. Phys, **134**, 044534.
17. Shaon Sahoo and **S. Ramasesha,** (2011) "Full spin and spatial symmetry adapted technique for correlated electronic Hamiltonians: Application to an icosahedral cluster", Int. J. Quantum Chem **112**, 1041 DOI 10.1002/qua.23097.
18. Simil Thomas, Anusooya Y, Pati and **S. Ramasesha**, (2011) "Nonlinear optical properties of stacked conjugated systems", Crystal Growth & Design, **11**, 1846.
19. Mousumi Das and **S. Ramasesha**, (2010) “Fluorescent resonant excitation energy transfer in linear polyenes”, J. Chem. Phys. **132**, 124109.
20. K. Hallberg, J. Rincon, M. Nizama, A.A. Aligia and **S. Ramasesha**, (2010) "Correlations, quantum entanglement and interference in nanoscopic systems", J. Stat. Mech: Theory and Expt., P11031.
21. Tirthankar Dutta and **S. Ramasesha**, (2010) “Double time window targeting technique: Real-time DMRG dynamics in Pariser-Parr-Pople model”, Phys. Rev. B **82**, 035115.
22. Manoranjan Kumar, Zoltan G. Soos, Diptiman Sen and **S. Ramasesha**, (2010) ‘Modified density matrix renormalization group algorithm for the zigzag spin ½ chain with frustrated antiferromagnetic exchange: Comparison with field theory at large J2/J1’, Phys. Rev. B **81,** 104406.
23. M. Kumar, S. Sarkar and **S. Ramasesha,** (2011) ”Supersolid Phase in 1-D Bose-Hubbard Model with Extended Range Interactions: DMRG and Field Theoretic Study at Different Densities”, Int. J. Mod. Phys. B **25**, 159 (arXiv:0812.5059).
24. Sukrit Mukhopadhya, **S. Ramasesha** and Suchismitha Guha, (2010) ‘Role of the triplet state in the green emission peak of polyfluorene films; a time evolution study’, J. Chem. Phys., **132**, 044104.
25. S. Mukhopadhyay, S**. Ramasesha**, S. R. B. Kanth and S. Patil, (2010) “Synthesis and characterisation of a class of donor-acceptor conjugated molecules: experiments and theory.” J. Phys. Chem A, **114**, 4647.
26. M. Kumar and **S. Ramasesha**, (2010) “A DMRG Study of the Low-Lying States of Transverse Substituted Trans-polyacetylene and Trans-polyacetylene”, Phys. Rev. B. **81**, 035115.
27. Thengarai S. Venkatakrishnan, Shaon Sahoo, Nicolas Bréfuel, Carine Duhayon, Carley Paulsen, Anne-Laure Barra, **S. Ramasesha**, Jean-Pascal Sutter, (2010) “Single-Chain Magnet behavior for a [{FeIIL}2{NbIV(CN)8}] Helical Chain Compound Designed with HeptacoordinateFeII”, J. Amer. Chem. Soc., **132**, 6047
28. M. Kumar, **S. Ramasesha** and Z. G. Soos, (2010) “ Bond-order wave phase, spin solitons and thermodynamics of a frustrated linear spin-1/2 Heisenberg antiferromagnet”, Phys. Rev. B 81, 054413
29. Z G. Soos, M. Kumar , **S. Ramasesha** , and R.A. Pascal, Jr., (2010) “1:1 alkali-TCNQ salts and the bond order wave (BOW) phase of half-filled linear Hubbard-type models”, conference paper, Physica B, **405** S353.
30. K. Hallberg, J. Rincon and **S. Ramasesha**, (2010) “Quantum transport through nanoscopic rings: charge-spin separation and interference effects”, Int. J. Mod. Phys. B, **24**, p5068.
31. J. Rincon, K. Hallberg, A.A. Aligia, and **S. Ramasesha** (2009) “Quantum interference in coherent molecular conductance”, Phys. Rev. Letts., **103,** 266807
32. M. Kumar, S. Sarkar and **S. Ramasesha,** (2009) ”Quantum Phase Analysis of 1D Superconducting Quantum Dot Lattice Using Extended Bose-Hubbard Model”, Euro Phys. J. **B72**, 503-507.
33. **S. Ramasesha**, Shaon Sahoo, Rajamani Raghunathan and Diptiman Sen, (2009) “Computing magnetic anisotropy constants of single molecule magnets”, J. Chem. Sci., **121**, 823.
34. S. Dhers, S. Sahoo, J.-P. Costes, C. Duhayon, **S. Ramasesha**, J.-P. Sutter (2009), “1-D hydrogen-bonded organization of hexanuclear {3d-4f-5d} complexes: Evidence for slow relaxation of the magnetization of [{LMe2Ni(H2O)Ln(H2O)4.5}2{W(CN)8}2] with Ln = Tb and Dy”, Cryst Eng Comm., **11**, 2078.
35. J.-P. Sutter, S. Dhers, R. Rajamani, **S. Ramasesha**, J.-P. Costes, C. Duhayon and L. Vendier (2009) “Heteo-metallic {3d-4f-5d} complexes: preparation and magnetic behavior of trinuclear [(LMe2Ni-Ln){W(CN)8}] compounds (Ln=Gd, Tb, Dy, Ho, Er, Y; LMe2=Schiff Base) and Variable SMM characteristics for the Tb derivative”, Inorg. Chem., **48**, 5820-5828.
36. M. Kumar, **S. Ramasesha** and Z. G. Soos (2009) “ Tuning the bond-order wave phase in the Half-filled extended Hubbard model”, Phys. Rev. B **79**, 035102.
37. M. Arif, S. Mukhopadhyay, **S. Ramasesha** and S. Guha (2009) “The role of triplet states in the emission mechanism of polymer light-emitting diodes”, Euro. Phys. Lett. **87**, 57008
38. S. Mukhopadhyay and **S. Ramasesha** (2009) “Study of linear and nonlinear optical properties of dendrimers using density matrix renormalization group method”, J. Chem. Phys. **131**, 074111.
39. P. Mahata, R. Raghunathan, D. Banerjee, D. Sen, **S. Ramasesha** , S. V. Bhat, and S. Natarajan (2009) “Fluorite and mixed-metal Kagome-related topologies in metal-organic framework compounds: synthesis, structure, and properties.” , Chemistry, an Asian Journal, **4**, 936-947.
40. S. Mukhopadhyay, B. J. Topham, Z. G. Soos, and **S. Ramasesha** , (2008) “Neutral and Charged Excited States in Polar Organic Films: Origin of Unusual Electro-luminescence in Tri-tolylamine-Based Hole Conductors”, J. Phys. Chem. A, **112**, 7271-7279.
41. M. Kumar, **S. Ramasesha**, R. A. Pascal Jr. and Z. G. Soos (2008) “ Dimerization transition of alkali TCNQ-salts: charge degrees of freedom near CDW boundary”, Euro. Phys. Lett., **83**, 37001 (Editor’s Choice Best of EPL 2008).
42. T.S. Venkatakrishnan, C. Desplanches, R. Raghunathan, P. Guionneau, L. Ducasse, S. **Ramasesha**, J.-P. Sutter (2008), “[{Ni(HL3)}2{W(CN)8}2] square: a case of antiferromagnetic {NiIIWV} interactions”, Inorg. Chem., **47**, 4854-4860.
43. R. Raghunathan, **S. Ramasesha**, C. Mathoniere, V. Marvaud (2008), “A kinetic model for photoswitching of magnetism in the high-spin molecule [Mo(IV)(CN)2(CN-Cu(II) (tren))6](ClO4)8”, Phys. Chem. Chem. Phys., **10**, 5469.
44. R. Raghunathan, **S. Ramasesha**, D. Sen (2008), “Theoretical approach for computing magnetic anisotropy in single molecule magnets”, Phys. Rev. B **78**, 104408.
45. S. Sahoo, R. Rajamani, **S. Ramasesha**, D. Sen (2008), “Fully Symmetrized Valence- Bond Based Technique for Solving Exchange Hamiltonian Molecular Magnets”, Phys. Rev. B **78**, 054408.
46. **S. Ramasesha**, R. Raghunathan (2007), “Multiscale Modeling of Molecular Magnets”, AIP Conference Proceedings, 963, 406.
47. Z. G. Soos, S. Mukhopadhyay, **S. Ramasesha**. (2007) “Polar organic films: Transport gap, charge-dipole interaction and electroluminescence of tritolylamine (TTA) derivatives”, Chem. Phys. Lett., **442**, 285-288
48. M. Kumar, **S. Ramasesha**, D. Sen, Z. G. Soos, (2007) “Scaling exponents in spin-1/2 Heisenberg chains with dimerization and frustration studied with the density-matrix renormalization group”, Phys. Rev. B. **75**, 052404.
49. Thengarai S. Venkatakrishnan, Rajamani Raghunathan, **S. Ramasesha**, J. –P. Sutter, (2007) “Synthesis, Crystal Structure, and Magnetic Properties of Hexanuclear [{MnL2}4{Nb(CN)8}2] and Nonanuclear [{MnL2}6{Nb(CN)8}3] Heterometallic Clusters (L = bpy, phen)”, Inorg. Chem., **46**, 9569.
50. **S. Ramasesha**, Rajamani Raghunathan, L. Ducasse, J.-P. Sutter, C. Mathoni`ere, (2006) ”Microscopic model for superexchange interactions and photomagnetism in binuclear transition metal complexes”, Phase Transitions, **79**, 637.
51. Rajamani Raghunathan, **S. Ramasesha**, Jean-Pascal Sutter, Laurent Ducasse, CedericDesplanches, (2006) “Microscopic model for high-spin vs. low-spin ground state in Ni2 M(CN)8 (M = MoV, WV , NdIV) magnetic clusters”, Phys. Rev. B **73**, 104438.
52. Sunil G. Naik, Arindam Mukherjee, RajamaniRaghunathnan, MunirathinamNethaji, **S. Ramasesha**, and Akhil R. Chakravarty, (2006) “Magneto-structural Study on a Tetracopper(II) Schiff Base Complex Stabilizing a Decanuclear Water Aggregate”, Polyhedron, **25**, 2135.
53. Rajamani Raghunathan, **S. Ramasesha**, Corine Mathoni`ere, Val´erie Mar-vaud, (2006) “Microscopic Model for Photoinduced Magnetism in the Molecular Complex [Mo(IV)(CN)2(CN − CuL)6]8+ Perchlorate”, Phys. Rev. B **73**, 045131.
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2. Sambunath Das, Dayasindhu Dey, Manoranjan Kumar and **S. Ramasesha**, “Quantum Phase Transition in Skewed Ladders: An Entanglement Entropy and Fidelity Study” (To be submitted).
3. Sambunath Das, Dayasindhu Dey, Manoranjan Kumar and **S. Ramasesha**, “Quadrupolar Phases and Plateau States in Skewed Ladders” (to be submitted).