CURRICULUM VITAE

Name: **Dr. Uttam Kumar Sinha Mahapatra**

Present official address: **Department of Physics**
Barasat Government College**, Barasat, 24 Pgs(N), India**
PIN: 700524

Present Designation: Associate Professor in Physics(West Bengal Educational Service)

Email: uttam.mahapatra@linuxmail.org

Date of Birth: **1st November, 1965**

Ph. D.(Sc): **Jadavpur University (Indian Association for the Cultivation of Science, Jadavpur)**

Title of the Doctoral Thesis: **Development of State-Specific Multireference Clu ster Expansion Approaches for Molecular Electronic States**

Supervisor**: Professor Debashis Mukherjee,**
Indian Association for the Cultivation of Science, Jadavpur,
Kolkata 700 032, India

Awards and Recognition:

- **Received the Siddhartha Sengupta Memorial Endowment Bronze Medal for First Position in Physics at the Master of Science examination, 1993.**
- **Awarded the UGC Junior Research Fellowship, 1993.**
- **GATE-93 WITH SCORE 91.58**
- **Awarded the Alexander von Humboldt Fellowship, Germany, 2001.**
- **Research Associateship Position at University of North Dakota, USA,2011 (not enjoyed)**

Educational Qualifications:

Name of Examination	Division	Year of Passing	Institutions / Universities
Madhyamik	1st	1981	West Bengal Board of Secondary Education
Higher Secondary	1st	1984	West Bengal Council of Higher Secondary Council
B. Sc. (Honours)	1st	1988	University of Burdwan
M. Sc.	1st **Rank: 1st**	1992*	University of Kalyani
Ph. D. (Science)		2000	Jadavpur University

***Examination held in 1993**

Professional career up to date in chronological order(list all appointments and posts held, nature of the work done)

Post held	Name of the Institution	Duration	Nature of work
Junior Research Fellow	Indian Association for the Cultivation of Science (IACS)	1994 – 1996	Doctoral Research
Senior Research Fellow	IACS	1996 – 2000	Doctoral Research work
Research Associate	IACS	2000 – 2001	Post-doctoral Research
Lecturer in Physics	Raiganj College	2001 – 2001	
Post Doctoral Fellow	University of Heidelberg, Germany	2001 – 2002	Post-doctoral Research
Lecturer in Physics	Darjeeling Govt. College	2002 –2006	Teaching UG students
Assistant Professor	Taki Government College	2006-2010	Teaching UG students
Associate Professor	Maulana Azad College	2010- 2019	Teaching UG students
Associate Professor	Barasat Government College	March, 2019- Till date	Teaching UG&PG students

Broad field of research interest with specific areas of involvement:

- **Theoretical Spectroscopy: Structure and Dynamics**
- **Many Body Quantum Theory of Atoms and Molecules: Relativistic and Nonrelativistic**

Visits abroad and nature of assignment: **Department of Theoretical Chemistry, University of Heidelberg, Germany, supported by a postdoctoral Fellowship of the *Alexander von Humboldt Foundation, Germany.***

Project

Completed: **DST (New Delhi):** Title of the Project "**Relativistic study of the excited/ionized states of heavy atoms using coupled cluster based linear response theory" [**Project No: SR/S1/PC-61/2009 Dated: 09.07.2011].

Completed: **DST (New Delhi):** Title of the Project **"Development and Applications of Intruder Free Multi-reference Perturbative and Non-perturbative Formalisms"** [Ref No. SR/SI/PC-32/2005].

Invited Talk: International symposium (Kodaikanal, India 28-31 January, 2009) on **"Recent Advances in Spectroscopy: Astrophysical, Theoretical and Experimental Perspective"**

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LIST OF RESEARCH PUBLICATIONS(1996-2017)

A: Journal Publications

1. Mitra, A., Sinha, D. and **Mahapatra, U. S.** (1996): "Open-shell coupled-cluster theory for a general incomplete model space using eigenvalue-independent partitioning", **Chem. Phys. Lett. 261**, 363-368.

2. **Mahapatra, U. S.**, Datta, B. and Mukherjee, D. (1998): "A state-specific multi-reference coupled cluster formalism with molecular applications", **Mol. Phys. 94**, 157-171.

3. **Mahapatra, U. S.**, Datta, B., Bandyopadhyay, B. and Mukherjee, D. (1998): "State-specific multi-reference coupled cluster formulations: Two Paradigms", **Adv. Quantum. Chem. 30**, 163-193.

4. Mitra, A., **Mahapatra, U. S.**, Majumdar, D. and Sinha, D. (1998): "Multiple solutions of coupled cluster equations: an application to molecular Auger spectra", **J. Phys. Chem. A 102**, 7277-7285.

5. **Mahapatra, U. S.**, Datta, B. and Mukherjee, D. (1999): "Development of a size-consistent state-specific multi-reference perturbation theory with relaxed model-space coefficients", **Chem. Phys. Lett 299**, 42-50.

6. **Mahapatra, U. S.**, Datta, B. and Mukherjee, D. (1999): "A size-consistent state specific multi-reference coupled cluster theory: formal developments and molecular applications", **J. Chem. Phys. 110**, 6171-6188.

7. **Mahapatra, U. S.**, Datta, B. and Mukherjee, D.(1999): "Molecular applications of a size-consistent state specific multi-reference perturbation theory with relaxed model space coefficient", **J. Phys. Chem. A 103**, 1822-1830.

8. Chaudhuri, R. K., Panda, P. K., Das, B. P., **Mahapatra, U. S.**, and Mukherjee, D. (1999): "Relativistic coupled-cluster-based linear response theory for ionization potentials of alkali-metal and alkaline-earth-metal atoms", **Phys. Rev. A 60**, 246-252.

9. Chattopadhyay, S., **Mahapatra, U. S.** and Mukherjee, D. (1999): "Property calculations using perturbed orbitals via state-specific multi-reference coupled cluster and perturbation theories", **J. Chem. Phys. 111**, 3820-3831.

10. Chattopadhyay, S., **Mahapatra, U. S.** and Mukherjee, D. (2000): "Development of linear response theory based on a state-specific multi-reference coupled cluster formalism", **J. Chem. Phys. 112**, 7939-7952.

11. Chattopadhyay, S., **Mahapatra, U. S.** and Mukherjee, D. (2000): "A Linear response theories for excited state energies for systems with strongly correlated ground state", **Ind. J. Chem. A (Special Issue on Contemporary Theoretical Chemistry Research in India) 39A**, 1-8.

12. Chaudhuri, R. K., Panda, P. K., Merlitz, H., Das, B. P., **Mahapatra, U. S.** and Mukherjee, D. (2000): "Relativistic Coupled--Cluster based Linear Response Theory for Ionization Potentials of Beryllium Like Ions**", J. Phys. B 33**, 5129-5138

13. Merlitz, H., Gopakumar, G., Chaudhury, R. K., Das, B. P., **Mahapatra, U. S.** and Mukherjee, D. (2001): "Core Effects on Ionization Potentials in Thallium", **Phys. Rev. A**, **63**, 022507-022510

14. Gopakumar, G., Merlitz H., Majumder S., Chaudhury, R. K., Das, B. P., **Mahapatra, U. S.,** and Mukherjee, D.(2001): "Ionization potential and Excitation Energy Calculations for Ba^+ using the Relativistic Coupled Cluster Method", **Phys. Rev. A**, **64**, 032502-032505

15. Jana D., **Mahapatra, U. S.** and Mukherjee, D. (2002): "A compact spin-free cluster expansion formalism for simple open-shell configurations", **Chem. Phys. Lett**., **353**, 100-110

16. Chattopadhyay, S., **Mahapatra, U. S.**, Datta, B. and Mukherjee, D. (2002): "State-specific multi-reference coupled electron-pair approximation like methods: formulation and molecular applications", **Chem. Phys. Lett., 356**, 426-433

17. Jana, D., **Mahapatra, U. S.**, and Mukherjee, D. (2002): "Use of a new cluster Ansatz to treat strong relaxation and correlation effects: A direct method of energy differences", **Int. J. Mol. Sc**., **3**, 550-569.

18. Majumder, S., Merlitz, H., Gopakumar, G., Das, B. P. **Mahapatra, U.S.**and Mukherjee, D. (2002)"Accurate calculations of interstellar lines of Mg+ using the coupled cluster approach" **Ap. J**. **574**, 513.

19. Gopakumar, G. Merlitz, H., Chaudhuri, R. K., Das, B. P., **Mahapatra, U.S.**and Mukherjee, D. (2002) "Electric dipole and quadrupole transition amplitudes for Ba¿ using the relativistic coupled-cluster method" **Phys. Rev. A**, **66**, 032505.

20. Sahoo, B. K, Chaudhuri, R. K. Das, B. P., Majumder, S., Merlitz, H., **Mahapatra, U. S.** and Mukherjee, D.(2003)" Influence of correlation effects on the magnetic dipole hyperfine interaction in the low-lying states of Ca+" **J. Phy. B**, **36**, 1899.

21. Chaudhuri, R. K., Shaoo, B. K., Holger, H., **Mahapatra, U. S.,** and Mukherjee, D. (2003)"Relativistic coupled cluster calculations of the energies for Rubidium and Cesium atoms**" J. Chem. Phys. 119**, 10633.

22. Sahoo, B. K., Gopakumar, G., Chaudhuri, R K , Das, B. P., Merlitz, H., **Mahapatra, U. S.,** and Mukherjee, D. (2003) "Magnetic dipole hyperfine interactions in $^{137}Ba^+$ and the accuracies of the neutral weak interaction matrix elements" **Phys. Rev. A 68**, 040501.

23. Chattopadhyay, S**.,** Ghosh, P., and **Mahapatra, U. S**. (2003) "Applications of Size-consistent State-specific Multi-reference Coupled Cluster (SS-MRCC) Theory to Study the Potential Energy Curves of Some Interesting Molecular Systems", **J. Phys. B. 37**, 495-510.

24. Chattopadhyay, S. and **Mahapatra, U. S. (2004)**: "Molecular Applications of State-specific Multi-reference Coupled Electron-pair approximation (SS-RCEPA)-like Method" **J. Phys. Chem A., 108, 11664-11678.**

25. Chattopadhyay, S., Pahari, D., **Mahapatra, U. S**. and Mukherjee, D. **(2004)**: "A State-Specific Approach to Multi-Reference Coupled Electron-pair Approximation like Methods: Development and Applications", **J. Chem. Phys, 120, 5968-5986.**

26. Majumder, S., Gopakumar, G., Chaudhuri, R. K., Das, B. P., Merlitz, **Mahapatra, U. S.** and Mukherjee, D. **(2004)** "Theoretical studies of electric quadruple transition probabilites in MG II" **Euro. J. Phys. D**. **28**, 3.

27. Nayak, M. K., Chaudhuri R. K., Chattopadhyay, S., and **Mahapatra, U. S. (2006)** "Core and Core-valence Extensive Coupled Cluster Theory and its Applications" **J. Mol. Struct. (Theochem) 768, 133-140.**

28. Chattopadhyay, S., **Mahapatra, U. S.** and Chaudhuri R. K., **(2007)** "Study of avoided curve crossing of an isolated 1:1 $AlHe^{+3}$ complex using many-body perturbation theory: A multi-reference approach" **Indian J. Phys. 81 1023-1037. [*Invited Article*]**

29. Chaudhuri, R. K., Freed, K. Chattopadhyay, S**.,** and **Mahapatra, U. S**, **(2008)** "Potential energy curve for isomerization of N2H2 and C2H4 using the improved virtual orbital multireference Møller–Plesset perturbation theory" **J. Chem. Phys. 128,** 144304

30. **Mahapatra, U. S**, Chattopadhyay, S**.** and Chaudhuri, R. K. **(2008)** "Molecular applications of state-specific multi-reference perturbation theory to HF, H_2S, C_2 and N_2" **J. Chem. Phys. 129,** 024108

31. Chaudhuri, R. K., Hammond J., Freed, K. Chattopadhyay, S**.** and **Mahapatra, U. S**, (**2008)** "Reappraisal of ***cis*** effect in 1, 2-dihaloethenes: An improved virtual orbital (IVO) multi-reference approach" **J. Chem. Phys. 129,** 064101**.**

32. Mahapatra, U. S, **Chattopadhyay, S.** and Chaudhuri, R. K. **(2008) "**Application of state-specific multi-reference Moller-Plesset perturbation theory to nonsinglet states" **J. Chem. Phys. 129**, 244108**.**

33. Chattopadhyay, S., Chaudhuri, R. K. and **Mahapatra, U. S, (2009)** "Application of improved virtual orbital based multireference methods to N_2, LiF, and C_4H_6 systems" **J. Chem. Phys. 130**, 014101**.**

34. Chattopadhyay, S. **Mahapatra, U. S,** and Chaudhuri, R. K. **(2009) "**Investigation of low-lying states of oxygen via second order multi-reference perturbation theory: A state-specific approach" **J. Phys. Chem. A 113**, 5972.

35. Chaudhuri, R. K., Chattopadhyay, S., **Mahapatra, U. S.** and Freed, K. **(2010)** "Molecular applications of analytical gradient approach for the improved virtual orbital-complete active space configuration interaction method" **J. Chem. Phys. 132**, 034105.

36. **Mahapatra, U. S.**, Chattopadhyay, S. and Chaudhuri, R. K. **(2010) "**Study of the ground state dissociation of diatomic molecular systems using state-specific multireference perturbation theory: A Brillouin-Wigner scheme" **J. Chem. Theo. Comp. 6**, 662.

37. **Mahapatra, U. S.**, Chattopadhyay, S. and Chaudhuri, R. K., **(2010)** "Second-Order State-Specific Multireference Møller-Plesset Perturbation Theory (SS-MRMPPT) Applied to Geometry Optimization" **J. Phys. Chem. A, 114**, 3668

38. Chattopadhyay, S., **Mahapatra, U. S.** and Chaudhuri, R. K., **(2010)** "Study of equilibrium geometries of diradicaloid systems via state specific multireference Moller-Plesset perturbation theory (SS-MRMPPT)" **Chem. Phys. Lett. 488**, 229

39. Chattopadhyay, S**.,** Chaudhuri, R. K. and **Mahapatra, U. S**, **(2010)** "Studies on *m*-benzyne and phenol via improved virtual orbital complete active space configuration interaction (IVO-CASCI) analytical gradient method" **Chem. Phys. Lett. 491**, 102.

40. **Mahapatra, U. S.** and Chattopadhyay, S. **(2010)** "Potential energy surface studies via a single root multireference coupled cluster theory" **J. Chem. Phys. 133,** 074102 (2010).

41. Mahapatra, U. S., **Chattopadhyay, S.** and Chaudhuri, R. K., **(2011)** "Second-order state-specific multireference Moller–Plesset perturbation theory (SS-MRMPPT): Application to energy surfaces of diimide, ethylene, butadiene and cyclobutadiene" **J. Comp. Chem. 32**, 325.

42. **Mahapatra, U. S** and Chattopadhyay, S. **(2010)** "Evaluation of the performance of single root multireference coupled cluster (sr-MRCC) method for ground and excited states, and its application to geometry optimization" **J. Chem. Phys.**, **134**, 044113.

43. Das, M., Chaudhuri, R. K., Chattopadhyay, S**.,** and **Mahapatra, U. S (2011)** "Valence universal multireference coupled cluster calculations of the properties of indium in its ground and excited states" ***J. Phys. B: At. Mol. Opt. Phys.*** **44** 065003**.**

44. **Mahapatra, U. S** and Chattopadhyay, S. **(2011)** "Application of an uncoupled state-specific multireference coupled cluster (UC-SSMRCC) method to a weakly bonded system: exploring the ground state ***J. Phys. B: Atomic, Molecular and Optical Physics*** **44**, 105102.

45. Das, M., Chaudhuri, R. K., Chattopadhyay, S**., Mahapatra, U. S.** and Mukherjee, P. K., **(2011)** "Application of relativistic coupled cluster linear response theory to helium like ions embedded in plasma environment" ***J. Phys. B: Atomic, Molecular and Optical Physics*** **44** 165701.

46. Chaudhuri, R. K., Chattopadhyay, S., K. F. Freed, and **Mahapatra, U. S**. **(2011)** "Economical description of static correlation for large systems (free base porphin and Mg-porphin complexes): An improved virtual orbital-complete active space configuration interaction (IVO-CASCI) analytical gradient method" ***J. Chem. Phys.*** **135**, 084118.

47. Chattopadhyay, S**.,** Chaudhuri, R. K., and **Mahapatra, U. S. (2011)** "Ab initio multireference investigations of disjoint diradicals: Singlet versus triplet ground state" ***Chem. Phys. Chem*****. 12**, 2791.

48. Das, M., Chaudhuri, R. K., Chattopadhyay, S., and **Mahapatra, U. S (2011)** "Fock space multireference coupled cluster calculations of the hyperfine structure of iso-electronic of $^{33}S^-$ and $^{35,37}Cl$" ***Phys. Rev. A*****. 84**, 042512

49. Chattopadhyay, S**., Mahapatra, U. S.** and Chaudhuri, R. K., **(2012)** "State specific multireference Møller--Plesset perturbation theory: A few applications to ground, excited and ionized states" ***Chem. Phys.*** **401**, 15. **Invited Article for Special Issue on "*Recent advances in electron correlation methods and applications*".**

50. **Mahapatra, U. S** and Chattopadhyay, S. **(2012)** "Single reference coupled cluster calculations for the weakly bound alkaline-earth dimers in the ground state" ***Mol. Phys*****. 110,** 75**.**

51. Chattopadhyay, S., **Mahapatra, U. S**. and Chaudhuri, R. K. **(2012)** "State specific complete active space multireference Møller-Plesset perturbation approach for quasidegenerate situations:Illustrating the bond breaking in hydrogen halides" ***Theo. Chem. Acc.*** **131,** 1213.

52. **Mahapatra, U. S** and Chattopadhyay, S. **(2012)** "Diagnosis of the performance of the state-specific multireference coupled-cluster method with different truncation schemes" ***J. Com. Chem.*** **33**, 1285**.**

53. Chaudhuri, R. K., Chattopadhyay, S., Freed K. F., **U. S. Mahapatra** (**2012)** "Theoretical aids in screening candidates for atomic clocks: illustration for Yb II" ***EuroPhysics Lett.*** **98,** 23002.

54. Chaudhuri, R. K., Chattopadhyay, S., Freed K. F., **U. S. Mahapatra** (**2012)** "Spectral lines behavior of Be I and Na I isoelectronic sequence in Debye plasma environment" **Phys. Plasmas 19**, 082701.

55. Chaudhuri, R. K. Chattopadhyay, S., and **Mahapatra, U. S. (2013), "**Taming the electronic structure of lead and eka-lead (E114) by the relativistic coupled-cluster method**"** ***J. Phys. Chem. A*** **117**, 8555. ***Invited Article in*** **Special Issue:** ***"Structure and Dynamics: ESDMC-2013"***

56. Chaudhuri, R. K., Chattopadhyay, S., Freed K. F., **U. S. Mahapatra** (**2013)** "Teoretical studies of the ground and excited state structures of stilbene" ***J. Phys. Chem. A 117, 9424. Invited Article*** in **Special Issue**: "***Oka Festschrift: Celebrating 45 Years of Astrochemistry".***

57. Chaudhuri, R. K., Chattopadhyay, S., **U. S. Mahapatra** (**2013)** "Reappraisal of nuclear quadrupole moments of atomic halogens via relativistic coupled cluster linear response theory for the ionized process" **J. Phys. Chem. A 117**, 12616**.**

58. **Mahapatra, U. S** and Chattopadhyay, S. (2013) "Binding in Beryllium Dimer: Contingent on the effects of electron correlations" **Science Journal**, MAC, Issue I**.**

*59 Chattopadhyay, S., **Mahapatra, U. S.** and Chaudhuri, R.K(2014), Dissociation of homonuclear diatomic halogens via multi-reference coupled cluster calculations, Mol. Phys. Vol 112, 2720*

*60 Sinha Mahapatra U, Banarjee D. Chaudhuri R. K. (2015) Profiling the binding motif between Be and Mg in the ground state via a single-reference coupled cluster method, Mol. Phys, **113, 1387***

*61 Chattopadhyay, S. Chaudhuri, R. K., U. S. Mahapatra (2015)*Sta**te-**specific multireference perturbation theory with improved virtual orbitals: Taming the ground state of F2, Be2, and N2 ***J. Com. Chem. 36, 907***

62. ***Ghosh Anirban, Chaudhuri Rjat K, Chattopadhyay Sudip, Sinha Mahapatra Uttam (2015) Relativistic State-Specific Multireference Perturbation Theory Incorporating Improved virtual orbitals: application to the ground state single-bond dissociation. J. Com. Chem 36 1954***

63.Chattopadhyay, Rajat K Chaudhuri, Uttam Sinha Mahapatra, Anirban Ghosh and Suvonil Sinha Ray(2016) State-specific multireference perturbation theory: development and present status. *Wiley Interdisciplinary Reviews: Computational Molecular Science* **6**:3, 266-291. (I. F. 10.23)

*64. Banerjee D., Mondal Monosij, Chattopadhyay S and Sinha Mahapatra Uttam.(2016) A state - specific multireference coupled -cluster approach with a cost- effective treatment of connected triples: implementation to geometry optimisation. Molecular Phisics, Molecular Physics 2016; **114**: 1591.*

65. Sinha Roy S., Chosh, S Sinha Maha Patra Uttam Chaudhuri Rajat K, and Chattopadhyay S, (2017) Combined complete active space configuration interaction and perturbation theoryapplied to applied to conformational energy prototypes:Rotation and inversion barriers. Computational and Theoretical Chemistry , 56,1120

B: Publications in Edited Books/Monographs

1. **Mahapatra, U. S.**, Datta, B. and Mukherjee, D. (1997): "A state-specific multi-reference Coupled Cluster Approach for treating Quasi-degeneracy", in *Recent Advances in Coupled-Cluster Methods*, Ed. Bartlett, R. J. (World Scientific, Singapore), 155-181.

2. Chattopadhyay, S., **Mahapatra, U. S.** and Mukherjee, D. (1999): "Response theories based on a state-specific multireference coupled cluster formalism", in *Recent Advances in Multireference Methods*, Ed: Hirao, K. (World Scientific, Singapore) 65-93.

3. Chattopadhyay, S., **Mahapatra, U. S.,** Ghosh, P. and Mukherjee, D. **(2002)**: "State-specific Multi-reference Coupled-cluster Based Methods for potential energy surface and their Approximate Variants", in ***Low-Lying Potential Energy Surfaces*****,** M. R. Hoffmann and K. G. Dyall Eds. (ACS Symposium Series No. 828, Washington, DC) **109-152**.

4. Pahari, D., Chattopadhyay, S., Das, S., Mukherjee, D. and **U. S. Mahapatra (2005)**: "Size-consistent State-specific Multi-reference Methods: A Survey of Some Recent Developments" in ***Theory and Applications of Computational Chemistry: The First 40 Years,*** Ed. C. F. Dykstra, *et. al* (Elsevier), **581-633**.

5. Chattopadhyay, S., Pahari, D., **U S Mahapatra**, and Mukherjee, D. **(2005):** "Computation of excited states potential energy surface via linear response theories based on state-specific multi-reference coupled electron-pair approximation like methods" in *Computational Chemistry: Reviews of Current Trends.* Ed. J Leszcynski (World Scientific, Singapore, New Jersy).

6. **Mahapatra, U. S.** and Chattopadhyay, S. **(2010) "**State specific calculation of dissociation potential energy curve using multireference perturbation theory**"** in "***Recent Advances in Spectroscopy: Astrophysical, Theoretical and Experimental Perspective***" (**Springer**).