1.	Name and address	Dr. Sourav Pal, FNA, FASC, FNASc, FRSC Director and Professor, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur-741246, Nadia, West Bengal
2.	Date and place of Birth	12th May 1955; Ranchi
3.	Address with telephone/Fax/e-mail No., etc	Dr. Sourav Pal IISER Kolkata Director's Bungalow, Mohanpur-741246, Nadia, West Bengal e-mail s.pal@iiserkol.ac.in
4.	Area of specialization	Theoretical Chemistry/ chemical physics

5.Academic Qualifications (Bachelor's degree onwards with University, year and subject)

Sr. No	Degree	Subject	Class/ CGPA	Year	University	Additional Particulars
1	M.Sc(Integrated-5yrs)	Chemistry	Ist Class	1977	Indian Institute of Technology (Kanpur)	
2	Ph.D	Chemistry		1985	IACS (Calcutta)	under the supervision of Prof. Debashis Mukherjee
3	Post-Doc Research Work	Quantum Chemistry		April '86 to Oct. '87	University of Florida, Gainesville, FL,USA	with Prof. R.J.Bartlett

6.	Field of specialization	Theoretical Chemical Physics with specialization in quantum chemistry; Computational Material Science

7. **Professional Experience**:

Presently Director and Professor, Chemistry, Indian Institute of science education and Research Kolkata from October 12, 2017
Professor (HAG) and Institute Chair Professor, Department of Chemistry, Indian Institute of Technology Bombay from June 1, 2015 to October 11, 2017 (Presently on depuation)
Scientist, CSIR- National Chemical Laboratory, Pune from Dec 9, 1982 till May 31, 2015
Head, Physical and Materials Chemistry, NCL, Pune, from December 2002 till Nov 30, 2010
Director, CSIR- NCL, Pune from December 1, 2010 till May 31, 2015

Director (Additional Charge), CSIR- Central Salt & Marine Chemicals Research Institute, Bhavnagar (Gujarat) from June 1, 2014 till May 31, 2015

Others: Adjunct Professor, Indian Institute of Science Education and Research, Pune from 2006 onwards
Distinguished Visiting Professor, Indian Institute of Technology, Kharagpur for five years from 2016

8. **Present Position**: Director, Indian Institute of Science Education and Research
Kolkata
On deputation from Department of Chemistry, Indian Institute of Technology (IIT) Bombay, Powai, Mumbai 400076

Former-President, Chemical Research Society of India

9. **Special Fellowship/ visiting appointment**:

J C Bose National Fellowship of DST, India

National Science Talent Search Scholar, 1972

Alexander von Humboldt Fellowship in Germany from Nov ’87 to March ’88, Sept’91 to Dec’91 and April’94 to August ’94, May, 2000 to July, 2000.

Visiting Professor at the Institute for Molecular Sciences, Okazaki, Japan from March, 1997 to September, 1997

Visiting Professor in University of Torun, Poland, November 2015

Distinguished Visiting Professor of Indian Institute of Technology, Kharagpur for a period of five years, from 2016.
Visiting Professor, Gauhati University

Visiting Scientist at the University of Arizona, Tucson, May 1995

“Dai-Ichi Karkaria Ltd” Endowment Fellow for 2004-05 by UICT, Mumbai

10. Awards and Honours

Special issue of Molecular Physics(an international journal at the interface between chemistry and physics) published in my honour on 60th birthday in the year 2015 (http://www.tandfonline.com/toc/tmph20/113/19-20)

- Recipient of the Shanti Swarup Bhatnagar Prize in Chemical Sciences, 2000
- Elected as Executive Council Member editor of Publications) of the Federation of Asian Chemical Societies (FACS)
- Served as President, Chemical Research Society of India (CRSI) from April 1, 2014 to March 31, 2017
- Recipient of SASTRA-CNR Rao Award in Chemistry & Materials Science for the year 2014
- Recipient of JC Bose National Fellowship of DST, 2008
- Recipient of Chemical Research Society of India Silver Medal, 2009
- Delivered Charles A Coulson Lecture Lecture in University of Georgia, USA, Feb 14, 2014
- Recipient of Professor Sadhan Basu Memorial Lecture Award of INSA, New Delhi, 2014
- Recipient of RPG Life Sciences Padma Vibhushan Prof M M Sharma Medal and Chemcon Distinguished Speaker Award , 2014
- Elected as a Fellow of the Indian National Science Academy, New Delhi, 2003
- Elected as a Fellow of the National Academy of Sciences, India, Allahabad, 1998
- Elected as a Fellow of the Indian Academy of Sciences, Bangalore, 1996
- Elected as a Fellow of the Royal Society of Chemistry, 2011
- Elected as a Fellow of West Bengal Academy of Science & Technology, 2011

- Received Dr. Jagdish Shankar Memorial Lecture of the Indian National Science Academy, 2006
- Recipient of Bimla Churn Law memorial Lecture Award of IACS, Kolkata, 2005
- Dai-Ichi Karkaria Endowment Fellow of UICT, 2004-05
- Recipient of the Chemical Research Society of India medal, 2000
- Elected as a Fellow of the Maharashtra Academy of Sciences, 1994
- Recipient of the NCL Research Foundation Scientist of the year (1999) award
- Recipient of the P.B.Gupta Memorial lecture Award of the Indian Association for the Cultivation of Science, Calcutta for 1993
- Received Council of Scientific and Industrial Research (CSIR) Young Scientist award in Chemical Sciences for 1989
- Received Indian National Science Academy (INSA) medal for Young Scientist 1987
- Received NCL Research Foundation Best Paper Award in Physical Sciences for the year 1995, 1996, 1997, 1999, 2000, 2002
- Delivered Prof. R. P. Mitra Memorial Lecture, Delhi University, 2010
- Delivered Prof. N.R.Dhar Memorial Lecture, 2011, University of Allahabad, 2011
- Recipient of "Science Councillor" Award -2011 of The Indian Society of Health, Environment, Education & Research (ISHEER) Jodhpur centre

11. **Membership of Editorial Boards of Journals / Societies**

- Nominated to be a member of the Editorial Advisory Board of The Journal of Physical Chemistry from Jan 1, 2018 for a period of three years.
- Chosen as a member of the Editorial Board of International Journal of Molecular Sciences from 2000
- President, Chemical Research Society of India from April 1, 2014 for three years
- Member, Editorial Board, Internationl Journal of Chemistry
- Member Advisory Editorial Board, Current Physical Chemistry, Bentham Science from 2010
- Member, Editorial Board, Journal of Chemical Sciences, published by the Indian Academy of Sciences, Bangalore from 2004
- Member, Editorial Board, Proc. Indian National Science Academy, from 1st January, 2006
- Member, Editorial Board, International Journal of Applied Chemistry, from 2005.
- Elected as a Life Member of the Society for Scientific Value

- Invited to be a Member, American Chemical Society for three years from 2015

12. Membership of important Committee

- Executive Council Member of the Federation of Asian Chemical Societies (FACS), from 2016
- Member of the Council of Indian National Science Academy from Jan 1, 2018 for three years
- Former President, Chemical Research Society of India, 2014-17
- Chairman, Chemical Division Council of Bureau of Indian Standards from June 2014
- National Representative of India in International Society for Theoretical Chemical Physics
- Member DST FIST (Chemical Science) committee from 2016 for a period of four years
- Member, School Board of school of Chemistry, University of Hyderabad
- Member, Research Advisory Council (RAC) in GAIL (India) Limited from 1-1-2012 onwards
- Member, Board of Governors, Academy of Scientific and Innovative Research (AcSIR)
- Special Invitee of the Board of Governors of IISER, Pune for a period of 3 years from 2013
- Member of Executive Council and Awards Selection Committee of ICC for the year 2011- present
- Member, screening & selection of NASI Scopus Young Scientist Awards 2012- 2014
- Member of National Advisory Committee of ISMC-2014, BARC, Mumbai
- Convener, Sectional Committee for the Chemical Sciences of Indian National Science Academy, New Delhi, 2013- 2015
- Member, Fellowship Scrutiny Committee (Physical Sciences), NASI, Allahabad 2014 - onwards
- Convener, Sectional Committee , Indian Academy of Science, Bangalore 2010-2012
- Member and Chairman of several project and human resource committee of CSIR EMR for more than ten years
- Member/Chairman of many important scientific award committee
- Member, Board of Director, CSIR Tech
- Chairman, NCL Venture Center

- Member, Governing Council, CWPRS, Pune
- Member, Working Group for XIIth five-year plan, Ministry of Environment & Forests
- Member, Working Group for XIIth five-year plan, Ministry of Environment & Forests
- Member, Working Group for XIIth five-year plan on high performance computing
- Invited Member, Working Group for XIIth five-year plan on higher education
- Member, Working Group for XIIth five-year plan on Chemical & Petrochemicals

13. **Work done**:

Contributions have been made to the diverse areas of theoretical chemical physics and span the intellectually demanding and challenging aspects of methodological and conceptual developments with an eye to applications to chemical problems. Following are the specific areas and details of the work carried out:

A: Frontier Theoretical Development on Molecular Electric Properties

Highly accurate theories have been developed by us taking into account the complex, correlated motion of electrons in molecules for the description of nonlinear electric properties. These theories using many-body coupled-cluster methods are based on the evaluation of derivatives of energy with respect to external fields in an analytic manner. Extensive development of these theories was done for molecules, which have closed shell configurations. The codes have been developed after extensive testing. The codes have potential use in the description of nonlinear molecular materials, with possible applications in electronic devices.
At the next stage, the more demanding cases of open shell systems, which are marked by high degree of quasi-degeneracy were addressed. This creates physical problems, which are theoretically difficult to address. Using a multi-determinant description of reference space, which can address this quasi-degeneracy adequately, coupled-cluster analytic derivative was formulated to compute accurate nonlinear properties. This general-purpose analytic derivative formulation is the first one based on multi-reference coupled-cluster method and is a significant development in quantum chemistry. We have implemented the theory to study properties of radicals and excited states. Excitation energies, ionization energies using the highly accurate multi-reference descriptions of coupled-cluster theory have also continued for a long

time. Recently, we have also developed first codes for transition dipole matrix elements using Fock space coupled-cluster theory.

B: Theoretical Investigation of Hard-Soft Acid-Base Relation

Qualitative principle related to hardness and softness has recently attracted a lot of attention in chemistry, in particular, due to the role of these in the explanation of stability of chemical species and reactivity. Our group has made early contribution by an extensive ab initio verification of the principle of maximum hardness. In particular, we have identified that for asymmetric distortions of molecules, the hardness is locally maximum. Various properties of hardness and softness were studied in relation to molecular properties, like polarizability. Using these relations, we could identify some novel relations between dipole moments and polarizability. Also among the recent contributions are use of local concepts of hardness and softness to chemical reactivity. Seminal contributions have been made by us in developing new local descriptors for intra- and inter-molecular reactivities. Recently, using local hard-soft-acid-base principle, interaction energies have been calculated with the help of only local descriptors of the interacting systems. We have recently identified “Bond Deformation Kernel” (BDK) correlating with interaction-induced shifts in O-H frequencies in halide-water clusters. Central to our model is the use of local polarization, which can be described by Normalized-Atom-Condensed Fukui Functions (NFF), which is the normal condensed Fukui Function multiplied by number of atoms. Using the NFF and charge transferred to water from halide ion, a BDK has been defined, which appropriately describes the shift in OH frequency

C: Study of Electron - Molecule Scattering

We have also made an important study in identifying the exchange effects as dominant contributions to the correlated static exchange (CSE) potential of the molecule in electron-molecule scattering. The properties of CSE were studied extensively in relation to their use in scattering of electrons by molecules.
Recently we have used complex-scaling method within the coupled-cluster method to describe the electron-atom resonance. A complex absorbing potential based and an approximation to this based on multi-reference coupled-cluster method to calculate resonance of molecular anions has also been developed. The procedure is based on the analytical continuation method. The advantage of analytical continuation of the Hamiltonian in the complex plane giving the direct access to the resonances parameters is that they can be represented by using L^2 wave function. The essential idea underlying the complex absorbing potentials to calculate the resonances is to introduce an

absorbing boundary condition in the exterior region of the molecular scattered target which results in a non-Hermitian Hamiltonian, one of the square-integrable eigenfunctions of which corresponds to the resonant state. The associated complex eigen-value then gives the position and width of the resonance or the auto-ionizing state. The important relaxation and correlation effects are included in the coupled-cluster method. The approximation developed in this year involves use of complex correlated independent particle potential, which simplifies the computation scheme. In the CIP –FSMRCC method, the analytical continuation over an already correlated effective Fock space Hamiltonian has been applied. We have tested this procedure to shape resonance in C_2H_4, CO and Mg. Recently, complex absorbing potential based equation-of-motion coupled-cluster theory has also been developed by us, which has been applied to shape resonance as well as inter-atomic couloumbic decay.

D: Application of Computational material Science

We developed ab initio molecular dynamics using Gaussian basis sets and Born-
Oppenheimer approximation to study reactions of finite-sized molecules. The Gaussian
basis sets are quite useful for finite sized molecules. In particular, we are studying
reactions inside finite clusters of zeolites and structures of metal clusters. Our study on structure and electron localization function of mixed metal clusters has led to the novel evidence of anti-aromaticitiicity in metal clusters.
Sn-beta zeolite has attracted recent interest due to better catalytic behaviour compared to Ti-Beta zeolite. Al-free Sn-beta zeolite has been recently synthesized and it has been shown by another group to have efficient catalytic activity in Beyer-Villeger oxidation reactions in presence of H_2O_2. At NCL, the structure, bonding and acidity of Sn-beta zeolite has been studied using periodic DFT and it has been demonstrated that incorporation of Sn in BEA framework reduces the cohesive energy and is n endothermic process. It has been also shown that among the T-sites, T2 site is the most probable site for Sn-incorporation. T2 site is also higher Lewis acid site in comparison to other T-sites. Theoretical analysis done at NCL also shows that Sn-atom polarizes the orbitals of oxygen atoms.
Several catalytically important bare as well as doped gold clusters and aluminum clusters have been identified for reactions. Special example of oxygen dissociation, CO-chemisorption and CO-oxidation has been highlighted using gold and silver clusters and the doped versions of these. Aluminum clusters have been used for important problem of nitrogen activation recently.

Computational study of reversible hydrogen storage materials, like magnesium hydrides using Born Oppenheimer molecular dynamics has been made. In particular, study of hydrogen desorption and the effect of dopants, Al and Si has been made. In recent years, we have studied the effects of dopants in form of metal ions and metal atoms to improve the hydrogen storage properties of metal-organic frameworks. Recent interesting work points to the scandium decorated MOF as a potential candidate for room temperature hydrogen storage material.

E. Density functional response approach for molecular properties:

A computationally viable alternative to full analytic response to Kohn-Sham density functional theoretic (DFT) approach, which solves coupled-perturbed Kohn-Sham (CPKS) procedure in non-iteratively has been formulated. In the above procedure, the derivative of KS matrix is obtained using finite field and then the density matrix derivative is obtained by single-step CPKS solution followed by analytic evaluation of properties. This has been implemented in deMON2K software and used for calculation of electric properties

F. Magnetic properties:

Recently, we are interested in calculation of magnetic properties of molecules using extended coupled-cluster method, which has been used successfully by us for electric property calculations. Specifically, this is used for evaluation of diamagnetic and paramagnetic susceptibility of closed shell systems. We are also working on use of multi-reference based coupled-cluster theories for open shell systems.

G Applications to interesting chemical problems

We have used our expertise as well as standard quantum chemistry techniques to important problems in chemical physics. One of the application areas has been the area of catalysis. Using various techniques, the modeling of catalytic properties of zeolites was addressed by energy calculation as well as use of concepts of hardness and softness. Weak inter-molecular interactions between small organic and inorganic molecules was also addressed. We are engaged in the application to the following areas:
Structure and spectra of medium sized organic molecules by ab initio method
Molecular modeling of structure and reactivity of zeolites
Semi-empirical method to determine structure and reaction of organic and organo-
 metallic systems

14. **Invitations to Conferences**

Delivered several (more than 150) invited lectures at several International and Indian Conferences. The most notable ones being the following:

Delivered an invited lecture at NCCP, 2017, Assam University, Silchar

Delivered an invited lecture at Current Trends in Theoretical Chemistry, Krakow, Poland, 2016

Delivered an invited lecture in Chemical Frontiers, Goa, 2016

Delivered an invited lecture at Asian Chemical Congress, Dhaka, March, 2016

Delivered an invited lecture at University of Torun, Poland, Nov 2015

Delivered an invited lecture at Recent Advances in Electron Structure Theory (RAEST), satellite of International Congress on Quantum Chemistry (ICQC), Nanjing, China, 2015

Delivered an invited lecture in ICCP9, National University of Singapore, 2015

Delivered an invited lecture in Department of Physics, University of Torun, Poland, 2015

Delivered an invited lecture at World Association of Theoretical and Computational Chemistry (WATOC), Santiago, Chile, 2014

Delivered invited lecture on School on DFT and beyond, M S University, Vadodara, 2014

Delivered an invited lecture in the International Conference on Education in Chemistry, HBCSE, Mumbai, 2014

Delivered an invited lecture in Edinburgh India Foundation Symposium, Edinburgh, 2014

Delivered Charles A Coulson Lecture , University of Georgia, Athens, USA, 2014

Delivered Plenary lecture, Sanibel Symposium, 2014

Delivered an invited lecture at Current Trends in Theoretical Chemistry (CTTC)-2013, BARC, Mumbai, September, 2013

Delivered an invited lecture in the European Materials (EUROMAT) conference in Sevilla, Spain, September, 2013

Delivered a key note lecture at Current Trends in theoretical Chemistry, Krakow, Poland, September, 2013

Delivered an invited lecture in Chemical Frontiers, Goa, August, 2013

Delivered an invited lecture in a conference on high performance computing at CSIR-CMMACS, Bangalore, August, 2013

Delivered a keynote lecture in a conference on Mapping Material Genomics, Shiv Nadar University, UP, March 2013

Delivered an invited lecture in SOCNAM, Jaipur (organized by Central University of Rajasthan), March 2013

Delivered an invited lecture in a conference on New Emerging Trends in Chemistry, IIS University, March 2013

Delivered an invited lecture in Spectroscopy and Dynamics of Molecules and Clusters, Udaipur, Feb 2013

Delivered an invited lecture on Electronic Structure and Dynamics of Molecules and Clusters, Kolkata, Feb 2013
Delivered a plenary lecture in 100th Indian Science Congress, Kolkata, January 2013
Delivered an invited lecture in Indo-French seminar on Energy materials, Paris, France, November 2012
Delivered an invited lecture in University of Florida, Gainesville , Fl, USA, October 2012
Delivered an invited lecture in Indo-UK conference (RSC) on Molecular Materials, held in London , September 2012
Delivered an invited lecture in Indo French workshop on catalysis, in Lille, France, July 2012
Delivered an invited lecture in the deMon workshop and Hearus Summer school held in Jacobs University, Bremen, Germany, July 2011
Delivered Plenary talk in the Second international Conference on Experiment-Integrated Computational Chemistry of Multi-scale Fluidics, held in Sendai, Japan, 23-24 February, 2010
Delivered invited lecture in International Conference on Recent Advances in Many-Electron Theory, Shankarpur, January, 2010
Delivered invited lecture in International Conference on Molecules and Materials, IISER, Kolkata, December, 2009
Invited Speaker in Indo-German conference on Dynamics of Excited States in Molecules, Dusseldorf, September, 2009
Invited Speaker in Indo-German conference on MCBR -2, Wildbad Kreuth, October, 2009
Invited speaker at International Workshop on Computational Material Science, Fuzhou, China, November, 2009
Invited speaker in International Conference on Simulations and Dynamics for Nanoscale and Biological Systems, Tokyo, 2009
Plenary lecture at the Sanibel Symposium, Georgia, USA, 2008
Invited speaker at QSCP XIII, Michigan, USA, 2008
Keynote speaker at CTTC V, Krakow, Poland, 2008
Invited speaker at International Workshop on Computational Material Science, Cairo, 2008
Invited lectures at two satellite conferences of the International Congress on Quantum Chemistry in 1994 and 1997.
Keynote lecture at the International Conference on Computational Methods in Science and Engineering, Attica, Greece, 2004
Invited lecture at the First Asian Pacific Conference on theoretical and computational Chemistry, Okazaki, Japan, 2004
Invited lectures at the density functional theory workshop of demon group in Paris, France, 2007, Dresden, Germany, 2005 and Calgary, 2006
Invited lecture International Conference on Computational Methods in Science and Engineering (ICCMSE), Loutraki, Greece, 2005, Corfu, Greece, 2007

Delivered a keynote talk in Symposium on Advanced Methods of Quantum Chemistry and Physics, 2007 at Torun, Poland, , 2007
Plenary speaker at Sanibel Symposum, St. Augstine, Florida, 2003

Chairs in major conferences:
Chaired a session on molecular properties at Molecular Quantum Mechanics (MQM) 2013, in honour of Rodney Bartlett, Lugano, June 2013
Invited to act as Session Chair/ Discussion Leader in the Conference on 'Molecular Quantum Mechanics: Analytic Gradients and Beyond' at Budapest, 30 May-3 June, 2007 and Invited as Chair in a workshop on coupled-cluster theory, a satellite meeting of the 9th International Congress on Quantum Chemistry, held at Cedar Key, Florida, USA in June 1997.
Chaired several other sessions at International Conferences

15. **Books Authored:** Co-authored a book " Mathematics in Chemistry" with Dr. K
V. Raman, Vikas Publishing House Pvt Ltd., New Delhi, 2004

16. **Special lectures**: Plenary speaker in 100th Indian Science Congress, Kolkata, 2012 and Inaugural keynote address in 6th Bihar Science Conference, Patna, 2014

17 . **Publications:** About 265 published papers in reputed international journals. Many of these are highly cited works. (Complete list of publications attached from next page as Appendix-1).

18. **Projects undertaken:**
Completed successfully several projects from DST, BRNS, IFCPAR, CSIR.
Completed successfully international projects: Indo-EU FP7 project, Indo-Slovak, indo-French (2 projects), Indo-Mexico
Presently having a collaborative with Indo- Mexico project
In addition, conducted contract research with companies in India and abroad, namely
Hindusthan Lever, Alchemie India, BASF, Germany and PPG, USA.

19. PhD Guided

Guided already about 32 Ph D students and currently another 10 students are working towards completion of Ph Ds.

Appendix-1

List of Publications of Dr. Sourav Pal in standard refereed publications

Name of the authors (year)	Title of the Paper	Name of Journal , Vol & Pg.No
1. M.D Prasad, Sourav Pal and D. Mukherjee (1980)	An alternative definition of the electron propagator in the super operator form and its relation to linear response theory	Pramana, 15, 531-543
2. Sourav Pal, M.D.Prasad and D.Mukherjee (1982)	On certain correspondences among various coupled cluster theories for closed shell systems	Pramana, 18, 261-270
3. M.D.Prasad, Sourav Pal and D.Mukherjee (1982)	Use of modified Propagators in many body perturbation theory	J.Chem.Soc(Faraday II),78,1743-1752
4. Sourav Pal, M.D.Prasad and D. Mukherjee (1983)	Use of size-consistent energy functional in many electron theory of closed shells	Theor.Chim.Acta, 62, 523-536
5. Sourav Pal (1984)	A variational method to calculate static electronic properties	Theor.Chim.Acta, 66,151 –159
6. Sourav Pal (1984)	Use of a unitary wave function in the calculation of static electron properties	Theor.Chim.Acta, 66, 207-215
7. Sourav Pal, M.D Prasad and D. Mukherjee (1984)	Development of a size-consistent energy functional for open shell states	Theor.Chim.Acta, 66, 311-332

8. M.D.Prasad, Sourav Pal and D.Mukherjee (1985)	Some aspects of self-consistent propagator theories	Phys.Rev.A 31,1287 -1298
9. Sourav Pal, M.D.Prasad and D.Mukherjee (1985)	A variational coupled cluster theory for closed shells using a propagator modification procedure	Theor.Chim.Acta., 68,125-138
10. Sourav Pal (1985)	Study of approximate coupled-cluster methods for first order static properties	Theor.Chim.Acta.,68, 379-388
11. Sourav Pal (1986)	Analysis of coupled-cluster methods for first order static properties	Phys.Rev.A, 33, 2240-2244
12. Sourav Pal (1986)	Bivariational coupled cluster approach for study of static properties	Phys.Rev.A.34, 2682-2686
13. Sourav Pal, M.Rittby, R.J.Bartlett, D.Sinha and D.Mukherjee (1987)	Multireference coupled-cluster methods using an incomplete model space : Application to ionization potentials and excitation energies of formaldehyde	Chem.Phys.Lett. 137, 273-278
14. K.B.Ghose and Sourav Pal (1987)	Bivariational coupled-cluster method: Equation for first order property	Phys.Rev.A 36,1539-1542
15. Sourav Pal, M.Rittby, R.J.Bartlett, D.Sinha and D.Mukherjee (1987)	Multireference coupled-cluster methods using an incomplete model space : Application to ionization potentials and excitation energies of Formaldehyde(E)	Chem.Phys.Lett ,142,575
16. Sourav Pal, M.Rittby , R.J.Bartlett, D.Sinha and D.Mukherjee (1988)	Molecular applications of multireference coupled-cluster methods using an Incomplete model space	J.Chem.Phys.,88,4357-4365
17. Sourav Pal (1989)	Multireference coupled cluster response approach for the calculation of static properties	Phys.Rev.A,39,39-42
18. Sourav Pal (1989)	Linearized bi variational coupled cluster approach: General scheme for the derivation of static properties	Phys.Rev.A39,2712-2714

19. M.Rittby, Sourav Pal and R.J.Bartlett (1989)	Multi reference coupled cluster method : Ionization potentials and excitation energies of ketene and Diazomethane	J.Chem.Phys.,90,3214 –3220
20. R. Mattie, M.Rittby, Sourav Pal and R.J.Bartlett (1989)	Applications of multi reference coupled cluster theory	Lect.Notes in chemistry, (Springer Verlag),50, 143-153) Ed.D.Mukherjee
21. Sourav Pal, M.Rittby, R.J Bartlett (1989)	Multi reference coupled cluster methods for ionization potentials with partial inclusion of triple excitations	Chem.Phys.Lett.,160,212-218
22. H.D.Meyer and Sourav Pal(1989)	A band-Lanczos method for computing matrix elements of a resolvent	J.Chem.Phys.,91,6195 –6204
23. D. Mukherjee and Sourav Pal (1989)	Use of Cluster expansion methods in the open shell correlation problem	Advances in Quantum Chemistry, 20,291-373
24. Sourav Pal(1990)	Coupled-cluster response approach: An improved variational strategy	Phys.Rev.A.,42, 4385-4387
25. R.Vetrivel, Sourav Pal and S.Krishnan(1991)	Property of iron containing ZSM-5 zeolite: A theoretical study based on quantum chemical calculations	J.Mol.Catal.,68, 385-397
26. K.B.Ghose and Sourav Pal(1991)	Multiple perturbation approach: Bounds to various order response	Chem.Phys.Lett.,187,637 –641
27. V. V. Bhate, A. D. Bhusari and Sourav Pal (1991)	Parallel ab initio quantum chemistry calculations on transputers	Advanced Computing, Ed. V. Bhatkar
28. Sourav Pal(1992)	An open shell coupled cluster response approach for static properties	Inter.J.Quantum.Chem., 41, 443-452,
29. Sourav Pal and K.B.Ghose (1992)	Analysis of coupled-cluster approach for higher order static properties	Phys.Rev.A,45,1518-1522

30. A.D.Bhusari, V.Bhate & Sourav Pal(1992)	Parallelization of molecular electronic structure calculation	Current Science, 62, 293-297
31. K.B.Ghose and Sourav Pal(1992)	Multireference coupled-cluster calculations on CH^{2+}	J.Chem.Phys,97 ,3863-3864
32. H.D.Meyer, Sourav Pal & U.V.Riss(1992)	Inclusion of electron correlation for the target wave function in low energy e^- N_2 scattering	Phys.Rev.A.,46, 186-193
33. Sourav Pal and K. B. Ghose (1992)	Coupled-cluster approach for static properties	Current Science, 63, 667- 677
34. Pinak Chakrabarti and Sourav Pal(1993)	Difference in the energies of interaction at the binding sites in protein structure	Chem.Phys.Lett .,201,24-26
35. Sourav Pal, Nayana Vaval and R.K.Roy (1993)	The principle of maximum hardness: An ab initio study	J.Phys.Chem.,9 7,4404 –4406
36. Nayana Vaval, K.B.Ghose, Sourav Pal & D.Mukherjee (1993)	Fock space multi reference coupled-cluster theory : Fourth order correction to ionization potential	Chem.Phys.Lett .,209, 292-298
37. K.B.Ghose, Sourav Pal and H.D.Meyer (1993)	Correlated static exchange interaction calculation of e^- N_2 scattering using coupled-cluster technique	J.Chem.Phys.,9 9,945-949
38. K.B.Ghose, P.G.Nair & Sourav Pal (1993)	Implementation of stationary coupled-cluster response method	Chem.Phys.Lett .,211,15 –19
39. Sourav Pal, R.K.Roy, and A.Chandra (1994)	Change of hardness and chemical potential in chemical binding: A quantitative model	J.Phys.Chem.,9 8,2314-2317
40. Nayana Vaval, R.K.Roy and Sourav Pal (1994)	On stationary multi determinantal coupled-cluster response	Phys.Rev.A,49,1 623-1628
41. K.B.Ghose and Sourav Pal (1994)	Influence of bond length on variation of static exchange potential : A case study in e^- N_2 scattering	J.Chem.Phys.,1 00, 4712-
42. Nayana Vaval, K.B.Ghose ,P.G.Nair and Sourav Pal (1994)	Stationary coupled-cluster response: role of cubic terms in molecular properties	Proc.Ind.Acad.S ci.,106, 387-392

43. Nayana Vaval, K.B.Ghose and Sourav Pal (1994)	Nonlinear molecular properties using biorthogonal response approach	J.Chem.Phys,101, 4914-4919
44. R.K.Roy, A.K.Chandra and Sourav Pal (1994)	Correlation of polarizability, hardness and electro-negativity: Poly atomic molecules	J.Phys.Chem., 98, 10447 – 10450
45. R.K.Roy, A.K.Chandra and Sourav Pal (1995)	Hardness as a function of polarizability in a reaction profile	J.Mol.Struct. (Theo.Chem), 331, 261-265
46. Sourav Pal K.B.Ghose and H.D.Meyer (1995)	Electron correlation in target molecule in low-energy e^- N_2 scattering	Inter.J.Quantum .Chem., 55, 291-297
47. A.K.Chandra, Sourav Pal, Ajay C. Limaye & Shridhar R.Gadre(1995)	Structure, energetics and bonding of diacetylene complexes with Hydrogen Fluoride: A theoretical investigation	Chem.Phys.Letters, 247, 95-100
48. A.K.Chandra and Sourav Pal (1995)	Studies on diacetylene complexes with water and ammonia	Chem. Phys. Letters 241, 399-403
49. Sourav Pal and A.K.Chandra (1995)	Some novel relationships of polarizability with dipole moments	J.Phys.Chem,99 ,13865 –13867
50. R.K.Roy and Sourav Pal (1995)	Chemical Potential and hardness of open shell radicals : Model for the corresponding anions	J.Phys.Chem, 99,17822-
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