Curriculum Vitae of K.L. Sebastian

1 Personal Details

Name and address	Prof. K.L. Sebastian Honorary Professor, Department of Inorganic and Physical Chemistry Indian Institute of Science Bangalore 560012, India Professor and Dean R&D, IIT Palakkad

2 Present Position

Professor and Dean R&D, IIT Palakkad

3 Academic Qualifications

Degree	Subject	Institution	Year	Rank/distinction
B.Sc.(Special)	Chemistry	Kerala University	1970	First Rank
M.Sc.	Physical Chemistry	Calicut University	1972	First Rank
Ph.D.	Theoretical Chemistry	IISc., Bangalore	1976	

4 Postdoctoral research

i) University of Liverpool (1980-82)
ii) Chalmers Institute of Technology, Sweden (1982)
iii) AvH Fellow, University of Munich (1983-84 and 1993) with Prof. *Gerhard Ertl*.

5 Positions held

Position	Institution	Period
Lecturer	Calicut University	1976 to 1984
Reader	University of Calicut	1984 to 1984
Professor	University of Cochin	1984 to 1996
Professor	IISc	1996 to 2016
Amrut Modi Chair	Division of Chemical Sciences, IISc	2007 to 2010
J.C. Bose Fellow	IISc	2008 to 2018
Professor and Dean	IIT Palakkad	January 2017 onwards

6 Awards/Fellowships of Academies/Lectures:

1. Vice President, Indian Academy of Sciences (2016 to 2018)
2. J.C. Bose Fellowship of the Department of Science and Technology, Goverment of India (2008 - 2018)
3. M.V. Pylee Award for Outstanding Academician (2010).
4. Amrut Mody Chair Professorship in the Division of Chemical Sciences, Indian Institute of Science, Bangalore (2007 - 2010)
5. Elected Fellow of the Indian Academy of Sciences (1994)
6. S.S. Bhatnagar prize in chemical sciences (1995)
7. Elected Fellow of the Indian National Science Academy (2001)
8. M.N. Saha Memorial Lecture at Indian Association for Cultivation of Science, Kolkata (2005)
9. Swadeshi Sastra Puraskar (1995)
10. Linus Pauling Lecture of the MG University (1995)
11. R.P. Mitra Memorial Lecture at the Delhi University (2007)
12. K.C. Mathew Endowment lecture at Bishop More College, Mavelikara (two times, 1993 and 2002)
13. K.V. Thomas Endowment lecture at S.H. College, Thevara

14. Prof. Iyer Memorial Lecture at U.C. College, Alwaye

7 Honorory Positions

1. Was Member, Condensed Matter Theory Unit JNCASR, Bangalore.
2. Was Member, Centre for Condensed Matter Theory, IISc, Bangalore (upto 2008).
3. Visiting Scientist, Max Planck Institute for Polymer Research, Mainz, Germnay (April- May, 2011).
4. Visiting Professor, University of Milan-Bicocca (October, 2010).
5. Member, Asian Institute of Nanobiosciences, Pusan, Korea (2003-2005).
6. Visiting Scientist, National Institute for Advanced Industrial Science and Technology, Tsukuba, Japan, (2002-2003).

8 Administrative Positions

1. Vice President, Indian Academy of Sciences (2016-2018)
2. Chairman, Science Education Panel of the Academies (2015-2017)
3. Chairman, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore (2005-2008), one term, of three years
4. Head Department of Applied Chemistry, CUSAT (one year, 1990-91)
5. Has been a member of the Board of Studies in Chemistry of MG University (1984-87), CUSAT (several times), and also the chairman of the Board. Was a member of the Board of Studies in Chemistry of Calicut University.
6. Member of the Science Education Panel of the Indian Academy of Sciences, Bangalore (1998-2001)
7. Member of Faculty selection boards of IIT Roorkee, IIT Patna, IISER Trivandrum, and Univerisities in Kerala, IIT Kanpur, and several other Institutions.

9 Editorial Board Memberships

1. Journal of Theoretical and Computational Nanoscience (American Scientific Publishers) (2002-2007).

2. Pramana (Indian Academy of Sciences) (2002-2007).

3. Resonance (Indian Academy of Sciences) (2002- 2014). *Chief Editor* for three years (2012-2014).

4. Journal of Indian Institute of Science (2005-2007).

10 Seminars and Conferences

He has given seminars at several universities (too numerous to list) in India and abroad.

11 Mentoring of Students

Sebastian has mentored a large number of students, at various levels and most of them ($> 95\%$) have continued in research.

1. Number of students at Doctoral level: 18 (13 have graduated)

2. He has mentored a large number of students at the Masters level. Most have continued to do their Ph.D. Their list along with their present affiliation is given below. Typically these are students who are at the first or second year of their Masters degree and they spend about two months in the lab. Some have been supported by the Indian Academy of Sciences/IISc/JNCASR. Most of them have chosen to continue in Research. Number of students at the Master's level: 28

12 Teaching

1. Has taught a variety of topics in Physical Chemistry at the Master's level, for 19 years, at Calicut University and the Cochin University of Science and Technology.

2. Has taught a variety of courses at IISc from 1996. Given below are the titles of the courses that have been taught:

   - Mathematics for Chemists
   - Group Theory for Chemists
   - Quantum Dynamics
   - Quantum Mechanics
   - Quantum Chemistry part of the course Quantum Chemistry and Statistical Mechanics, offered to the Int. Ph.D. students
   - Statistical Thermodynamics
   - Physical Chemistry I
   - Physical Principles of Chemistry *(first chemistry course for the UG students)*

3. Has recorded **49 video lectures on Introductory Quantum Chemistry** under NPTEL. These are available for free download at Youtube.

13 Publications (General)

He has been very active in promoting science Education. This includes giving talks at various levels to teachers and students, and writing articles at a level that can be understood by under graduate and post graduate students, in the journal Resonance published by the Indian Academy of Sciences, Bangalore. His area of research is theoretical chemistry, which was very poorly taught in Kerala. He has given a large number of lectures to the teachers, enthusing them in the topic and theoretical chemistry is taught better now.

1. K.L. Sebastian: Electrons in Atoms, Shapes of Atomic Orbitals (a poster and commentary), Resonance, Vol. 2, 88 (1997)

2. K.L. Sebastian: Molecular Wheel Observed! Current Science, 75, 536 (1998).

3. K.L. Sebastian: Knots and Links, Resonance, April (2006)

4. K.L. Sebastian: Mechanochemistry: The Amazing Viral DNA Packaging Molecular Motor, Resonance, May 2007

5. G. Baskaran, C. Arunachalam and K.L. Sebastian: S.K. Rangarajan (1932-2008), Current Science, May 2008

6. R.S. Swathi and K.L. Sebastian: MolecularMechanism of Heterogeneous Catalysis. The 2007 Nobel Prize in Chemistry, Resonance, June 2008

7. K.L. Sebastian and R. de Levie: S.K. Rangarajan, a tribute, Journal of Electroanalytical Chemistry, Dec. 2008

14 RESEARCH CONTRIBUTIONS OF K.L. SEBASTIAN

K.L. Sebastian has worked on a variety of different problems in theoretical chemistry. His work is summarized below (in reverse chronological order):

14.1 Diffusion in Crowded Media

In usual diffusion processes, $< x^2(t) > \propto t$ and the probability distribution for the displacement of the particle is Gaussian. However, recently for diffusion processes happending in crowded and rearranging media, it has been found experimentally that the probability distribution function is exponential and not Gaussian. A model for this is to assume that the diffusion coefficient is changing stochastically as a function of time. We have found an analytically solvable model, for the model and this agrees quite well with the experimental observations. A variety of different ways in which the diffusion coefficient can change have been considered.

14.2 π-distortivity

Why is Bezene a perfect hexagon with D_{6h} symmetry? Controversy existed as to whether it is due to the π system of the σ system. Using the force approach, we provide unambiguous proof that the π system is distortive and that it is the sigma system that leads to the D_{6h} geometry.

14.3 Path Integrals for Levy Walks

Levy walks are generalizations of Brownian motion, which are currently a topic of great interest. In the past few months, we have developed a path integral approach for Levy walks, and used it to solve the following problems involving a particle undergoing Levy walks in the following constraints.

- Free
- Subject to a linear and harmonic potential
- Overdamped, subject to linear and harmonic potentials and time dependent forcing.

- Underdamped motion in linear and harmonic potential
- Kramers like problem

14.4 Coherence in the Photosystem

Recently, it has been experimentally demonstrated that quantum coherence is important in the energy transfer process in the photosystem of at least some organisms. The theoretical modeling of this is very difficult and the methods that have been used are very cumbersome. We have come up with an approach that gives an analytical solution to the problem.

14.5 Biophysical Chemistry

A very interesting problem that was solved by Sebastian *et al* is the generalization of the famous Kramers problem [1, 2, 3], to a long chain molecule surmounting a barrier. This problem has been referred to as "intractable" in the literature [4]. The problem is of considerable interest and importance and has been the subject of several papers [4, 8, 9]. A kink mechanism has been suggested and it is in agreement with the experimental results [10, 11]. For biological translocations, the transition state was found to have the shape of a hook, again in agreement with the accepted views in cell biology [9]

Motivated by the experiments on DNA under torsion, Sebastian considered the problem of pulling a polymer out of a potential well by a force applied to one of its ends. If the force is greater than a critical value [18, 19], then the process is barrier-less. Sebastian has used the Rouse model for the description of the dynamics and found that the time t_{po} required to pull out a polymer of N segments scales like N^2. For models other than the Rouse, he argues that $t_{po} \sim N^{1+\nu}$. Very recently, this was extended to cover the case where excluded volume effects are included by Sebastian *et al* in a very elegant paper [21].

Further, recently, there has been experimental work [22] on a long chain DNA molecule, that is being packaged in to a viral capsid. It has been possible to study the rate of packaging as a function of a pulling force exerted at its end. This has been analyzed by Sebastian's group and they have proposed a Butler-Volmer type equation for the description of kinetics [23].

Other processes for which interesting results have been obtained are: (a) breaking of a long chain molecule under tension and (b) opening of a weak

link in the polymer loop (c) translocation of a long chain molecule through a membrane, caused by adsorption of molecules on one side and (d) movement of proteins through the nuclear pore complex.

14.6 Flourescence Resonance Energy Transfer

Recently energy transfer for nano-sized systems has been studied theoretically. It had recently been found that the energy transfer from an excited dye to a gold nanoparticle has a distance dependence which is different from the expected R^{-6} behavior. The dependence was d^{-4} where d is the distance from the surface of the nanoparticle. We performed theoretical calculations and found that the energy transfer to electron-hole paris and plasmons lead to only R^{-6} dependence[25]. We also analyzed energy transfer to a sheet of graphene and found that it has a d^{-4} dependence[26]. This prediction has been experimentally cofirmed, and it has lead to a variety interesting applications in a number of papers (approximately 20 papers, by different authors, who have developed a variety of sensors). We have also predicted that this power law dependency will change over to an exponential one, if graphene is doped to sufficient extent, a prediction that is yet to be verified. Another prediction is that the rate of energy transfer to a carbon nanotube has a d^{-5} dependence.

14.7 Nanotechnology and Molecular Devices

A very interesting suggestion that has been made by the group of Sebastian is that hypostrophene molecule adsorbed on a surface, is a molecular roller [27]. They have also studied other systems like systems cyclopentadienyl attached to Ge, Si and Sn surfaces - these are examples of molecular wheels [28].

It has also been shown that cyclo-nonatetraenyllithium is a molecular rattle, in which the Li atom can go from one side of the ring to the other, through the ring. The dynamics of vibrational excitation in a single molecule transistor using C_{60} and showed that (a) the distance dependence of the hopping matrix element can be important and (b) non-planarity of the surface is important [30].

14.8 Reaction Dynamics on a Continuum of Potential Energy Surfaces

A chemical reaction, usually takes place on the ground state adiabatic potential energy surface and to calculate the rate one usually makes use of multidimensional quantum transition state theory. If any other surface plays a role in the reaction dynamics, then one includes a non-adiabaticity correction, for which a Landau-Zener type theory may be used [34]. However, if there are a continuum of intersecting potential energy surfaces, how would one take the non-adiabaticity in to account? This is quite an interesting problem and arises in the calculation of the rates of electrochemical reactions at the surface of a metal electrode, as the metal has a continuum of possible electronic excitations. It would also be of importance in catalytic reactions happening on the surface of a metal. The problem has been recognized long ago by Marcus[35], and had remained an unsolved problem. Sebastian has suggested a novel way of accounting for the electronic excitations, which is to treat them as bosons[36]. Using this procedure, he has calculated the rate of simple electrochemical electron transfer reactions, with non-adiabaticity accounted for. This is a very important contribution to the field of chemical reaction dynamics. This has lead to further interesting work in the field - see the paper by Smith and Hynes[37], which extends this work by using an improved model for the liquid, in the electrochemical electron transfer reaction. Sebastian has considered how this may be applied to applied it to the electrochemical proton transfer reaction [39].

14.9 Electrons at Surfaces

Recently Sebastian et al.[31] have looked at the solvation of an electron, trapped in an image potential state on the surface of a metal, by a layer of polar adsorbates. Using a simple model, it has been found that the electron can exist in a localized state, caused by the polarization of the adsorbates, or in a delocalized state. There can be a barrier between the two. For parameters which reproduce the experimental data, it was found that there is no barrier between the two. The dynamics of the solvation too was studied[32] using a trial wave function and was found to be in good agreement with experimental observations. The photoinduced electron injection into a semiconductor from a dye molecule adsorbed on its surface was studied in [33]. It was shown that the electronic part of the Hamiltonian can be

traced away and an effective non-Hermitian Hamiltonian can be obtained for the vibrational motion. This non-Hermitian Hamiltonian can be used to calculated vibrational excitation probabilties that result from the electron injection.

14.10 Dynamics of Barrierless Reactions

Another problem that is quite interesting is the dynamics of barrier-less reactions[40]. A simple model for such reactions would be a particle executing one-dimensional random walk on a harmonic potential, in presence of a delta function sink, located at some position[40]. An exact solution to this model was proposed by Sebastian[41, 42]. This has lead to further interesting and important work in the field. See reference [43] in which the method of solution is used extensively, to analyze a related problem (see also ref. [44]). Recently, the same technique has been used to solve the two dimensional version of the problem[45].

14.11 Adsorption of Polymers on Disordered Surfaces

The group of Sebastian has studied the statistical mechanics of the adsorption of polymers on surfaces. The usual approach to adsorption is to solve a diffusion equation, with a de Gennes boundary condition [46] to account for the attractive interaction between the solid and the polymer. A path integral approach to the problem appears difficult as one expects the paths (polymer conformations) to be constrained by the presence of the hard solid and hence unable to adopt configurations which penetrate into the solid. Sebastian and Sumithra showed how this may be removed, and how one can work with paths that are unconstrained, to analyze the problem. Using this, an analysis of the adsorption of polymer molecules on a disordered surface was made. It was found that as the disorder increases, the polymer molecule collapses in a direction parallel to the surface[47]. As the randomness increases, it was found to undergo a collapse in the perpendicular direction too, so that the molecule becomes a two dimensional object.

14.12 Principle of Maximum Hardness

The principle of maximum hardness states that molecules arrange their electronic structure so as to have the maximum possible hardness[48]. If true,

this is a very interesting concept and the principle has been claimed to have been proved rigorously[49]. Sebastian has shown that the proof is in error[50]. This point was missed by several authors [51] and is expected to change the current way of thinking on this topic.

14.13 Dynamical Effects in Tunneling

Sebastian has also been involved investigating dynamical effects in tunneling. It was found that dynamical image interaction can modify the barrier height for tunneling considerably, and that the effect was more important than believed earlier[52, 53, 54]. He has also studied the barrier height for tunneling in electrochemical scanning tunneling microscopy and found that solvent reorganization cannot happen during tunneling and hence the consequent lowering of the barrier height is negligible[54].

14.14 Time Dependent Coupled Cluster Theory

In addition to the above, he has studied the neutralization of an ion which is scattered from the surface of a metal using a time dependent version of the Newns-Anderson Hamiltonian. The procedure consists of solving for the matrix elements of the time evolution operator explicitly. Including coulombic repulsions make the problem a difficult many body one. For ions with closed shells one can get time dependent Hartree-Fock solutions. It was shown that this solution is defective in that it predicts the probability of neutralization to be less than 0.5. This means that correlation effects have to be included for a correct description of the process. In order to account for correlation effects, a time dependent version of the coupled cluster theory was used. Using this, neutralization probabilities for Li^+ ions scattered from the surface of Ni was calculated. Also the spectrum of excitations produced in the solid by the reflected ions have been calculated. This was one of the first development and application of time dependent coupled cluster to a genuinely time dependent problem [55, 56].

14.15 Path Integrals and Brownian Motion

Gaussian path integrals whose potentials are non-local in time arise in a number of problems in physics and chemistry. If the potential is local in time the result is known in an analytic form. Sebastian has derived a similar

expression for the non-local case and used it to evaluate the path integral involving Bezak's action [57]. Also, he have developed a procedure for evaluating a path integral involving a more general action than that of Bezak[57]. A useful model for polymers is to model them as paths followed by a particle executing Brownian motion. This analogy means that one can use averages over Brownian paths to calculate average properties of a polymer molecule. The average over a Brownian path can be represented as a path integral. It has been suggested that one can also model polymers in different regimes, using generalizations of Brownian motion, referred to as fractional Brownian motion (FBM). Sebastian has developed a path integral representation for FBM and used it to evaluate averages that are of interest to the polymer theorist[58].

14.16 Theory of Chemisorption and Electron Energy Loss Spectroscopy

Using the superoperator formalism, methods for going beyond the Hartree-Fock approximation for the Newns-Anderson Hamiltonian, as applied to chemisorption were found[59]. The method was applied to the chemisorption of an atom on a semi-infinite linear chain. Correlation effects were found to be of importance in determining the density of states on the atom and in describing the dissociation limits correctly[60]. In addition, a theory for vibrational excitation of adsorbate vibrations in electron scattering from surfaces was developed and used for calculations [61]. From this, an important selection rule, viz., only vibrations perpendicular to the surface can be excited by electrons scattered in the specular direction was arrived at [62].

References

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14. Publications in Journals

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