

## Curriculum Vitae of Dr. Rebecca Jacob

### Work Experience

Designation	Institution	Years	Duties
<b>Associate Professor</b> (2006 to 2007) <b>Reader</b> (1996 to 2005) <b>Selection Grade Lecturer</b> (1996) <b>Senior Lecturer</b> (1988-1996) <b>Lecturer</b> (1981-1988)	Department of Chemistry, <b>Madras Christian College</b> , Tambaram, Chennai, (Madras) 600 059, India. <a href="http://www.mcc.edu.in">http://www.mcc.edu.in</a>	<b>1981 to 2007</b> (Leave on loss of pay from 2000 to 2005). Rejoined in December 2005 & took voluntary retirement in October 2007.)	Teaching (70-80%) Research (10%) Administration (10-20%)
Visiting Fellow (2000) Post-doctoral Research Fellow (2001 - 2002)	<b>The Australian National University</b> , Canberra ACT 0200, Australia. <a href="http://www.anu.edu.au">http://www.anu.edu.au</a>	2000 to 2002	Research (90%) Teaching (10%)
Post-doctoral Research Fellow. (2003 -2006) Visiting Fellow (2006 - 2007)	Royal Melbourne Institute of Technology ( <b>RMIT University</b> ), Melbourne VIC 3001, Australia <a href="http://www.rmit.edu.au">http://www.rmit.edu.au</a>	2003 -2007	Research (75%) Supervision of students & Administration (20%) Teaching (5%)
Research Associate (November 2007 to June 2008)	Monash University (Clayton campus), VIC 3800, Australia. <a href="http://www.monash.edu.au">http://www.monash.edu.au</a>	2007-2008	Research
Casual Academic	Monash University La Trobe University RMIT University	2008	Mix of Research, teaching and demonstrating
Visiting Research Fellow.	La Trobe University <a href="http://www.latrobe.edu.au/">http://www.latrobe.edu.au/</a>	2009	Mix of Research, teaching and demonstrating
Casual Academic	University of Sydney Sydney, NSW 2006 Australia	2010 onwards	Mix of Research, teaching and demonstrating

**Work address:** Room 209 B, The School of Chemistry, The University of Sydney, NSW 2006

**Phone** +61 2 9351 5361 **Mobile** 0469798291

**Email:** [Rebecca.jacob@sydney.edu.au](mailto:Rebecca.jacob@sydney.edu.au)

**Web Page:** <http://groups.chem.usyd.edu.au/radom/People/index.html>

**Date of birth:** 27<sup>th</sup> of October 1958. **Nationality:** Australian

### Professional Memberships

1. Member of The Royal Australian Chemical Institute -Chartered Chemist [MRACI (C.Chem)]
2. Life member of The Chemical Research Society of India.
3. Life member of The Society for Polymer Science, India, Madras Chapter.

### Selected Publications

1. H and D Attachment to Naphthalene: Spectra and Thermochemistry of Cold Gas-Phase C<sub>10</sub>H<sub>9</sub> and C<sub>10</sub>H<sub>8</sub>D Radicals and Cations; Olha Krechkivska, Callan M. Wilcox, Bun Chan, Rebecca Jacob, Yu Liu, Klaas Nauta, Scott H. Kable, Leo Radom and Timothy W. Schmidt **Journal of Physical Chemistry A** 2015 (accepted for publication).
2. Mechanism of the dielectric enhancement in polymer–alumina nano-particle composites Rebecca Jacob \*, Anne Pavitra Jacob, David E. Mainwaring **Journal of Molecular Structure** 2009, **933(1-3)**, 77-85.
3. Synthesis, characterization and ab initio theoretical study of a molecularly imprinted polymer selective for biosensor materials; Rebecca Jacob\*, Margaret Glewis, Yididya Banti, Colin Rix and David E. Mainwaring **Journal of Physical Chemistry A** 2008, **112 (2)**, 322-331.
4. Rearrangements in model peptide-type radicals via intramolecular hydrogen-atom transfer: Damian Moran, Rebecca Jacob, Geoffrey P F Wood, Michelle L Coote, Michael J Davies, Richard A J O'Hair, Christopher J Easton, Leo Radom, **Helvetica Chimica Acta** 2006, **89(10)**, 2254-2272.
5. Bond Dissociation Energies and Radical Stabilization Energies Associated with Model Peptide-Backbone Radicals: Geoffrey P. F. Wood, Damian Moran, Rebecca Jacob, and Leo Radom **Journal of Physical Chemistry A** 2005, **109 (28)**, 6318 -6325.
6. The mechanism of the dissolution, spray and deposition technique - a novel infrared sampling method; Rebecca Jacob **Spectrochimica Acta Part A**: 2003, **59**, 1557 -1563
7. Infrared Spectra and Structures of the Valyl-Alanine and Alanyl-Valine Zwitterions Isolated In A KBr Matrix: Rebecca Jacob and Gad Fischer **Journal of Physical Chemistry A** 2003, **107(32)**, 6136-6143.
8. Infrared absorption spectra and structures of zwitterions of glycyl-L-alanine and its N-deuterated isotopomers in a KBr matrix: Rebecca Jacob and Gad Fischer **Journal of Molecular Structure** 2002, **613**, 175-188.
9. Towards Non-Vertical Radical Cations: Quantum Chemical Studies on Pentafulvene and Triafulvene Radical Cations: Rebecca Jacob\*, S.Viswanathan and E.J.Padma Malar, **Indian Journal of Chemistry** 2002, **41B**, 1923-192
10. Infrared Spectra and the Structures of the Valyl-Glycine Zwitterion Isolated in A KBr Matrix; Gad Fischer, Rebecca Jacob and Xiaolin Cao **Chemical Physics** 2001, **263**, 243-253.
11. Isotope Effects on the Equilibrium of p-Benzoquinone and its Radical Anion: Ab Initio and DFT Studies; Rebecca Jacob, Mrinalini Puranik and Jayaraman Chandrasekhar **Chemical Physics Letters** 1999, **301**, 498-502.
12. The Role of Lysine-41 in Rnase A Catalysis. A Quantum Chemical Study on the Active Site-Ligand Complex; Saraswathi Vishveshwara, Rebecca Jacob, Gautham Nadig, Jacob V Maizel JR ; **Journal of Molecular Structure** 1998, **471**, 1-11.

### Academic Qualifications

Exam Passed	University	Year	Class / Grade	Remarks
S.S.L.C	Kerala	1973	First Class	53rd Rank in the state out of 200,000 students
Pre-degree	Kerala	1975	First Class	First from the College in English and Chemistry.
B.Sc.	Kerala	1978	First Class	First from the College in Mathematics, English and Chemistry. 100% in Mathematics
M.Sc.	Madras	1981	A Grade	First from the College – the best out going post graduate student.
M.Phil.	Madras	1987		Thesis Entitled, “Kinetics of Alkaline Hydrolysis of 2,4-Pentanedione – Conductivity Method”
Ph.D.	Madras	1996		Ph.D. Thesis Entitled, “Computational Studies of Structures Energies and Properties of Radical Ions and Some Biologically and Industrially Important Molecules”

### Successful Grant Applications

Title	Funding agency and year received	Applicants	Amount in A\$
Molecularly imprinted films as pesticide and herbicide sensors.	GRDC, Vic Dept. of Agriculture and CRC-Viticulture. (2005 & 2006)	Prof. David Mainwaring, A/Prof. Colin Rix, Dr. Rebecca Jacob and Dr. Margaret Glewis. (RMIT University)	294,000
A molecular approach to the development of nanoscale diagnostic platforms for Hepatitis C	VPAC-Victorian Partnership for Advanced Computing E-research grant. (2005)	Prof. David Mainwaring, Dr. Rebecca Jacob, RMIT and Dr. David Chalmers, Medicinal Chemistry, Victorian College of Pharmacy, <b>Monash University</b> .	17,500
"What's in That? Exploring Chemistry Through Virtual Reality"	Victorian Institute of Chemical Sciences (VICS). 2005.	Dr. Rebecca Jacob, RMIT, A/Prof. Peter Tregloan, Chemistry School, <b>University of Melbourne</b> ; Dr. David Chalmers, Victorian College of Pharmacy, <b>Monash University</b> and Mr Sean Hart, VR Centre - ICubed, RMIT;	29,650
Ligand/Receptor binding studies using interactive force-field molecular dynamics.	VPAC-Victorian Partnership for Advanced Computing E-research grant.2003	Prof. David Mainwaring and Dr. Rebecca Jacob, RMIT University.	\$50,920

### Successful Computing Time Grants

**Service Provider: EMSL User Services, W.R. Wiley Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, P.O. Box 999, MS K8-84, Richland, WA 99352, USA [userservices@emsl.pnl.gov](mailto:userservices@emsl.pnl.gov) Phone: 509-376-2553 Fax: 509-376-6742**

Project Title	Applicant	Project code / user id	Year	Computing time
Molecular Modelling Studies of Molecularly Imprinted Polymers Selective for Biosensor Materials.	Rebecca Jacob, Applied Chemistry RMIT University	Proposal ID: 3630 User ID: 34172	2003	75,000 hours

### Australian Partnership for Advanced Computing (APAC) Merit Allocation Scheme Grants:

Project Title	Applicants	Project code	Year
Infrared Spectra and Structures of Di-peptide Zwitterions Isolated in a KBr Matrix	Rebecca Jacob, Department of Applied Chemistry, RMIT University	Project h61 RFCD Codes 250104, 250699	2005
Molecular Imprinted Polymers - Nature of the Molecular Recognition Mechanism	David Mainwaring and Rebecca Jacob, Department of Applied Chemistry, RMIT University	Project f20 RFCD Codes 250601, 250302, 250303, 250104	2003 2004 2005
Structural and Mechanistic Chemistry	Principal Investigator Leo Radom Co-Investigators Thomas Buesgen, Michelle Coote, David Henry, Rebecca Jacob, Anthony Scott, Michael Sullivan, Geoff Wood, Computational Quantum Chemistry, Research School of Chemistry, Australian National University. Ines Corral, Chemistry, Autonoma University of Madrid.	Project d39, k29 RFCD Codes 250699	2002 2003 2004 2005
Spectra and Molecular Structures	Gad Fischer and Rebecca Jacob Department of Chemistry, Faculty of Science, ANU	Project u01, u54 RFCD Codes 250104, 250105, 250699	2000 2001 2002

**Service Provider: Victorian Partnership for Advanced Computing (VPAC)**

Project Title	Applicants	Project code	Year
Molecular Imprinted Polymers	Project Supervisor: Rebecca Jacob, RMIT University	pRMIT0029	2005 2004 2003
<b>Partner Share Computational Projects grant on APAC and VPAC</b>			
A molecular approach to the development of nanoscale diagnostic platforms for Hepatitis C	Project Supervisor: Rebecca Jacob, RMIT University	Project h59 on APAC	2005
Understanding the Role of Molecular Interactions within the Interfacial Region of High Dielectric Nanocomposite Films for Flexible Microelectronics through Modelling.	D.E. Mainwaring, R. Jacob and P. Murugaraj, RMIT University	Project h60 on APAC	2003 2004

**What's in that?**

**“What's in that?”** is a large 3D virtual reality presentation that allows the user to see some of the dynamic molecular world underlying everyday life. It was developed as part of the Chemistry Outreach program of the Victorian Institute for Chemical Sciences (VICS), a collaboration between the University of Melbourne, Monash University and RMIT University.

I got the idea for this project soon after I joined RMIT University in 2003.

**"Chemistry through Virtual Reality – A Three Dimensional Molecular Modeling Presentation"** was submitted as a grant application to National Science week, RACI etc. Though the applications were not successful I got very positive feedback and hence I approached VICS with my idea. This program is a spectacular display, whereby the public is exposed to the mystery of chemistry. Making chemistry interesting, intuitive and interactive is the aim of this project. The audience is immersed into a virtual reality environment whereby they can see and interact with the molecules in 3D. For example, instead of telling them that water is H<sub>2</sub>O we actually show them the molecules. The relative sizes of the atoms are realistically depicted in the models and the molecules are modeled to replicate the original molecules, using different colours for the different atoms etc. Audiences attending such a presentation enjoy an interactive and entertaining educational experience whilst intuitively learning and understanding what chemistry is at the molecular level. It was a very novel idea at that time as 3-D technology was just developing.

**“What's in that?”** received very wide recognition. Its first public showings were at our 2006 open days. It was shown at all the three universities - University of Melbourne, Monash University and RMIT University and was very well received. A mobile version of the program was then created so that it could be taken to schools for programs with Year 9-12 students. This part was funded by the VICS outreach program.

The extension of this technology to other virtual environments and to versions of **“What's in that?”** for use in public places were explored. A range of real experiments and demonstrations for school students to complement the virtual molecular experience of **“What's in that?”** was investigated.

### **Successful Grant Application in India:**

A project for establishing facility for research in material science in the Department of Chemistry, Madras Christian College, Tambaram, Chennai was envisaged and a grant application was submitted to the **Department of Science and Technology (DST)**, Delhi, India. My experience and expertise in the field was the main basis for the application. This application was successful and we received (**Rs. 32, 00, 000**) thirty two hundred thousand rupees for this project in the year 2006. This is a very large sum of money to be won by an individual department of a college. We established and refurbished facilities in the lab including some structural modifications. One GC, IR and one DRIS UV-VIS spectrophotometer was purchased and about half a dozen PCs were installed. Using all these new facilities, our department is now involved in active research work. This was a major contribution I gave to MCC before I took my voluntary retirement in 2007.

### **Responsibilities at the University of Sydney**

#### **Research:**

I perform research in computational chemistry (theoretical calculations on organic systems and biological systems) with Pro. Leo Radom seven hours a week (20% pro-rata fellowship). I also co-supervised one student for her TSP (Talented Student Program) project in 2014.

#### **Lecturing:**

I have been teaching the University Preparation Course in Chemistry every year since 2010. This included 4 hours of lecturing per week as well as two three-hour lab sessions for six weeks. I prepare the course material, lecture all the classes, conduct the laboratory component of the course, set the question paper, mark the answer papers and finalise the mark list. The students get admitted into the University the subsequent year based on the successful completion of this course. I have been appointed on a continuing basis to teach the University Preparation Course in Chemistry every year. I also teach the HSC (High School Certificate) Preparation courses.

#### **Tutoring:**

Sydney University has a general tutorial session where an experienced tutor sits in a tutorial room from 1pm to 2pm. The students can come in and ask questions about any topic and the tutor helps them. The tutor has to be very knowledgeable in every branch of chemistry. I have been taking up this tutorial session every semester since 2010. We get around 2500 students doing first year chemistry every year and currently I am the only duty tutor.

I am the tutor for the elite athletes' program and for the indigenous students' program.

#### **Demonstrating:**

I have been demonstrating first year, second year and third year laboratory classes regularly every semester since the beginning of 2010.

#### **Bridging Course and Summer School**

Sydney University conducts bridging courses regularly. I am part of the team tutoring the bridging course since 2010. I also teach courses for the summer school.

### Special Distinctions

- 1) Received the University Grants Commission's teacher fellowship to do research from July 1993 to July 1994 at the Indian Institute of Science, Bangalore.
- 2) Received the Visiting Fellowship from the Jawaharlal Nehru Centre for Advanced Scientific Research in 1995.
- 3) Received the Young Scientist Fellowship sponsored by the Tamil Nadu State Council for Science and Technology in 1996.
- 4) Received the Fellowship from the Indian Academy of Sciences in 1997.
- 5) Holder of National Merit Scholarship throughout university education.
- 6) Scored 100% in Mathematics in the BSc degree final public examination.
- 7) Received a Certificate of Merit from the University of Kerala for dedicated service to the National Service Scheme in 1977.
- 8) Was the best out-going post-graduate student from Madras Christian College in 1981 and was absorbed into the Faculty of Chemistry immediately on passing out.
- 9) Successfully completed the course conducted by *Aptech Computer Education* in 1999.

### Papers in Preparation.

1. Infrared Absorption Spectra and Structures of Zwitterions Of Glycyl-L-Tryptophan and its N-Deuterated Isotopomers in a KBr Matrix Using a Novel Sample Technique: Rebecca Jacob.
2. Infrared Absorption Spectra and Structures of Phenolsulfonphthalein Dyes: Rebecca Jacob and Anne Pavitra Jacob.
3. UV spectra of carbon radicals and sulfur radicals. Benchmarking of DFT methods excited state energy calculations: Rebecca Jacob and Leo Radom.
4. Hydrogen transfer reactions in carbon radicals and sulfur radicals: Rebecca Jacob and Leo Radom.

### Research Skill

I have knowledge in a variety of computational methodologies such as molecular mechanics, semi-empirical procedures and ab initio methods. I have worked using Gaussian 92, 94, 96, 98 and 03 programs. I have acquired all the skills necessary for independently establishing a Computational Quantum Chemistry Research Group. I have performed theoretical calculations at very high levels like G3, G3MP2 Rad, G3-B3LYP etc as well as HF and DFT calculations. I am conversant in molecular modelling using INSIGHT II Biosym Software Packages for structural simulation. I am well versed in the use of the Schrödinger package that addresses the challenges in pharmaceutical research for structure-based drug design. I have performed accurate, rapid ligand-receptor docking using Glide. I have used Jaguar, the high-performance ab initio quantum mechanics application, and MacroModel, a versatile molecular modelling tool. I am proficient in Visual Molecular Dynamics (VMD), Molden, Molecule, Spartan, xfig and other similar molecular modelling programs and also graphical programs like Sigma Plot, Grams, Animol, Opus NT, Chemdraw etc. I have used numerous computer systems ranging from PCs, I860, and IBM workstations to mainframes using operating systems such as DOS, UNIX and WINDOWS as well as Macintosh machines.

I have been running calculations on the super computer systems of Australian Partnership for Advanced Computing (APAC) since 2000 and Victorian Partnership for Advanced Computing (VPAC) since 2003. I have worked on complex biological systems as well as small molecules.

I have experience in various experimental techniques like FTIR spectroscopy, Kinetics and Scanning Electron Microscopy. Besides handling practical classes for the students, I have done experimental work, mainly kinetics and some organic synthesis and analysis for my M.Phil and M.Sc thesis. I am also versatile in the use of numerous tools such as SciFinder Scholar and EndNote used in research, literature searches and writing journal papers.

### **University Teaching Experience in India**

I have held academic positions continuously since 1981, mainly teaching chemistry at the University level.

Madras Christian College (MCC), where I worked **since 1981**, was started in 1837 and is still reputed to be among the top ten colleges of India. With 700 universities and more than 35,000 affiliated colleges enrolling more than 20 million students, Indian higher education is a large and complex system. The quality of the educational institutions in India is judged by the quality of the graduates the institution produces, unlike Australian Universities where the ranking is based on the quality of the research of the academics. Most of the students who graduate from MCC join the work force immediately. There is a stiff competition from companies to grab the good students through campus interviews.

*India Today* the most popular news magazine of India publishes an annual survey ranking the top ten colleges in India and Madras Christian College has always maintained its position at the top of the list every year and obtained the first rank in Science in 2003. Being in the top 10 consistently for almost two decades is remarkable when we consider the fact that there are more than thirty five thousand colleges in India. MCC has always obtained a ranking of **A+** by the National Assessment and Accreditation Council (**NAAC**). Only very few educational institutions in India have an A+ ranking by NAAC.

M.C.C is a lush, wooded, campus situated on 400 acres of sprawling forests and gardens. The Indian Postal Service released a stamp in 1987 to commemorate the College's 150 years of success and academic standing. Our long list of outstanding alumni includes Dr. S Radhakrishnan, former president of India. Our college was among the first few institutions in India to be granted autonomy. This has led to the introduction of new courses, curricular innovations and examination reforms. Under such an autonomous pattern, I have been involved at different levels of planning and execution of both curriculum development and assessment of the students.

MCC is one of the best centers for higher education for undergraduate and postgraduate studies. We have an excellent textbook library in the chemistry department. As a permanent member of the faculty of chemistry of Madras Christian College since August 1981, I have been teaching physical chemistry for the post-graduate students and all the branches of chemistry for the graduate students. I am used to lecturing to a large number of students in huge lecture theaters. There are about 100 to 200 students attending a graduate lecture class. English is the medium of instruction at the university level in India.

I have guided several M.Sc. and M.Phil. students (about 2 or 3 each year) for their research projects and dissertations, in a variety of topics including organic and analytical chemistry, mostly in collaboration with local industries for more than two decades. These were mainly short-term projects geared up to introduce the students to the fundamentals of research methodologies.



I have been a member of the Board of Studies (which frames the syllabi for B.Sc. and M.Sc. students) since 1982 and the M.Phil. Board since 1989. I have been a member of the Board of Examiners, which scrutinizes the question papers and approve the examination results every semester, both at the graduate and postgraduate levels. I have set question papers; marked answer scripts and conducted end of semester laboratory practical examinations for B.Sc. and M.Sc. students (since 1982) and M.Phil. students (since 1989). I have conducted laboratory practical classes for the students (around 60 students in a laboratory class at the UG level and 15 to 18 students in a class at the PG level), training them in various analytical techniques, qualitative and quantitative analysis, as well as experiments involving the synthesis and purification of organic compounds, structural elucidation and detection of different functional groups, throughout my teaching career at MCC. I was on leave from MCC from 2000 to 2005. In December 2005 I returned to India, rejoined MCC and took voluntary retirement in October 2007.

### University Teaching Experience in Australia

I started my academic career in Australia from 2000 onwards. As Visiting Fellow, Department of Chemistry, Faculty of Science, The Australian National University, Canberra ACT 0200, Australia I taught part of the course CHEM 3105 (Selected Topics in Physical Chemistry) for the BSc (honours) third year students. At RMIT University I was the primary supervisor of the student Mr. **Harit Jani** for the project, “*Touch-enabled Visualization of molecular dynamics, using PHANToM Haptic Interface*” for his course Master of Engineering in Information Technology. He worked with me as a research assistant for two months and then joined me for his Ph.D. I was also one of the Ph.D. supervisors for Mr. Mohammad Al Kobaisi. I also taught under graduate courses when requested.

In 2008 I decided to free lance. To gain experience and exposure to a wide range of topics in academia, I performed a mix of teaching and research activities at different universities. I had taken up casual teaching positions at three different universities namely Monash University, La Trobe University and RMIT University handling first, second and third year students.

In 2010 I shifted to Sydney and I have been working as a casual academic staff at the University of Sydney. I do research in computational chemistry as well as undergraduate teaching.

### Research Experience

I registered for Ph.D. in January 1989 and worked under Dr. K Rengarajan, Professor, Department of Chemistry, Madras Christian College, and Dr. S Viswanathan, Professor, Department of Polymer Science, University of Madras, in Theoretical Physical Organic Chemistry [Computational Chemistry]. Research work was carried out part time, along with the normal teaching work load which is mandatory for a Lecturer in the affiliated colleges in India. Ph.D. thesis was submitted to the University of Madras in October 1995 and Ph.D. degree was awarded in August 1996.

I worked under the guidance of Dr. J Chandrasekar, Professor, Department of Organic Chemistry, Indian Institute of Science, Bangalore in Computational Chemistry spending all the summer vacations (April to June) and Christmas holidays doing research at The Indian Institute of Science (IISc) from 1991 onwards and the entire year from July 1993 to July 1994 under the University Grants Commission’s teacher fellowship, so as to complete Ph.D. Continued collaborative research work with Dr. J Chandrasekar under the Visiting Fellowship from the Jawaharlal Nehru Center for Advanced Scientific Research in 1995 and the Fellowship from the Indian Academy of Sciences in 1997 during the summer holidays. Dr. J Chandrasekar, was the winner of the Bhatnagar award, the highest award for a scientist in India (just like Nobel

prize is for the whole world). He is a fellow of the International Union of Pure and Applied Chemistry. <http://www.iupac.org/web/per/chandrasekhar>

I carried out collaborative research work with Dr. Saraswathi Vishveshwara, Professor, Molecular Biophysics Unit, Indian Institute of Science, Bangalore in 1996 with the Young Scientist Fellowship sponsored by the Tamil Nadu State Council for Science and Technology. The Young Scientist Fellowship is funded by the Department of Science and Technology (DST), India and is awarded annually to the best young scientist employed in any of the science, technology or engineering departments across all universities and research organizations. Dr. Saraswathi Vishveshwara, was a post-doctoral fellow of Prof John A Pople, Noble laureate in Chemistry.

The Indian Institute of Science (IISc) started in 1909 is a premier institution of research and advanced instruction, with more than 2000 active researchers working in almost all frontier areas of science and technology. It has a very high international standing in the academic world. <http://www.iisc.ernet.in/>. In the latest Quacquarelli Symonds (QS) World University Rankings announced on 17th September 2014 the **Indian Institute of Science (IISc), ranks eleventh globally** for high research output in the area of **citations-per-faculty**.

As Visiting Fellow at The Australian National University, I worked on the infra-red spectra of dipeptides (both experimental & theoretical) with Dr. Gad Fischer, Head of the Department of Chemistry, from April 2000 to February 2002 and completed several projects. I gained expertise in the use of the FT-IR Spectrometer. I also carried out scanning electron microscopy studies and even mass spectral analysis.

I worked with Prof Leo Radom in Theoretical Quantum Chemistry in The Research School of Chemistry, The Australian National University, Canberra ACT 0200, Australia, from February 2002 to December 2002. I finished several projects on hydrogen transfer in peptides using ab initio molecular orbital theory to investigate the possibility of backbone intramolecular hydrogen transfer in polypeptide radicals by building up models to replicate the mid chain environment in poly-glycine systems. We also studied the effect of intramolecular hydrogen transfer in polypeptide radicals using a model tetra-peptide system as well as intermolecular hydrogen transfer and base assisted intramolecular hydrogen transfer in polypeptide radicals.

I worked at the RMIT University, Melbourne VIC 3001 from 2003 to 2006. I have completed several projects on molecularly imprinted polymers selective for biosensor materials and two other projects (a) on polymer-metal oxide nanocomposites and (b) on the GFP-GFP dimer interactions. Most of the work performed here was industry funded and hence confidentiality agreements prevent us from presently publishing the results.

I returned to India in early 2006 and re-joined Madras Christian College. I guided several postgraduate students and my expertise enabled our department to get a substantial DST grant. I took voluntary retirement with full benefits from MCC in October 2007.

From November 2007 onwards, I worked as a Research Associate with Prof. Don McNaughton at Monash University (Clayton campus), VIC 3800, Australia in infrared spectroscopy investigating the effect of nasty substances like cyanides on food. In 2009 I joined a computational chemistry project with Dr David Wilson, Dept. of Chemistry, La Trobe University, Bundoora VIC, Australia.

In 2010 I shifted to Sydney and I do research in computational chemistry with Prof. Leo Radom at the University of Sydney. I have worked on a few projects and some are in the process of being written up.

### Conference Presentations

1. Infrared Absorption Spectra and Structures of Phenolsulfonphthalein Dyes: presented at Connect 2005, the 12th RACI National Convention held at Sydney Convention and Exhibition Centre, Darling Harbour Sydney NSW Australia from July 3-7, 2005.
2. Ab initio Theoretical Study of Molecular Imprinting Polymers Selective for Biosensor Materials: presented at the Australian Gaussian Workshop held at The School of Chemistry, The University of Sydney, Australia from June 28 - July 1, 2004.
3. Infrared Absorption Spectra, Structures and Conformations of Zwitterions of Glycyl-L-tryptophan and its N-deuterated Isotopomer in a KBr Matrix presented at MM2004, the 9th Molecular Modelling Workshop, a combined meeting of the Asia / Pacific Chapter of the MGMS, the Biomolecular Chemistry Division of the RACI and the Molecular Modellers in Australia held at the Intercontinental Hotel, Sydney, Australia from 30 June 2004 to 3 July 2004.
4. Molecular Dynamics Simulations with Three Dimensional Force Feedback presented at CPC2004: Conference on Physical Chemistry 2004, conducted by The Royal Australian Chemical Institute held at Hobart, Tasmania, Australia from 1-5 February 2004.
5. Molecular Modelling Studies of Molecularly Imprinted Polymers Selective for Biosensor Materials: paper presented at the International Conference on Computational Science 2003 (ICCS 2003) held at Melbourne, Australia from June 2 - 4, 2003.
6. The Infrared Spectra and Structures of the Zwitterions of Dipeptides Isolated in an Alkyl Halide Matrix: presented at the CPC 2002 Conference on Physical Chemistry 2002, at the University of Canterbury, Christchurch, New Zealand from 3-7 February 2002
7. Conformations, Structures and Infrared Spectra of Dipeptide Zwitterions : presented at the World Chemistry Congress 2001, held at Brisbane, Australia from July 1 - 6, 2001.
8. Computational Study of The Redox Behaviour of p-Benzoquinone : Through Space and Through Bond Interactions, presented at the National Symposium in Chemistry held at the Indian Institute of Chemical Technology, Hyderabad during January 27 – 29, 2000.
9. Quantum Chemical Investigations on Some Reactant Molecules Used for the Synthesis of Polymale-amides, presented at the National Seminar on Polymers For The New Millennium conducted by The Society for Polymer Science, India, Madras Chapter at The University of Madras, Chennai during March 25 – 26, 1999.
10. Computational Studies on FK506 presented at the UGC sponsored National Seminar on Recent Trends in Chemical Research held at Gurunak Dev University, Amritsar during March 22 – 23, 1999.
11. Computational Studies on Some Organic Molecules Useful For Polymer Industry, presented at the National Conference on Chemistry Industry and Environment (N.C.C.I.E – 99) held at P G Department of Chemistry, Government College, Rajahmundry, Andhra Pradesh during February 25 –27, 1999.
12. Towards Non-Vertical Radical Cations: Studies On Pentafulvene And Triafulvene Radical Cations presented at the National Symposium in Chemistry held at the Indian Institute of Science, Bangalore during January 27 – 30, 1999.
13. Long Range Interactions in Radical Ions presented at The Chemists Meet held at The Indian Institute of Technology, Madras during December 3 - 4, 1997.

14. Possible Non-Classical Structures for Ethane Radical Cations and Isoelectronic Species – A Computational Study presented at The Chemists Meet held at The Indian Institute of Technology, Madras during December 12 – 14, 1996.
  15. Radical Cations of Strained Hydrocarbons- A Study of Norbornadiene Quadricyclane Systems and Semibullvalene Systems presented at the National Symposium on New Vistas in Chemical Sciences during March 19 –20, 1996.
  16. Molecular Mechanics Calculations on Phenol-sulphonphthalein Dyes presented at the UGS-DRS National Seminar on New trends in Dynamic and Structural Studies in Inorganic and Physical Chemistry, at The School of Chemistry, Madurai Kamaraj University, Madurai, Tamil Nadu during March 1 – 3, 1995.
  17. Molecular Mechanics Calculations on FK506 presented at the eleventh conference of Indian Council of Chemists at L. S. College, Muzaffarpur, Bihar during March 12 - 14, 1993.
  18. Kinetics of Oxidation of Camphor by N-Bromo-Succinimide presented at the National Seminar on Applications of Physical Methods in Chemistry held at Annamalai University, Annamalai Nagar, Tamil Nadu from March 17 - 19, 1989.
  19. Kinetics of Alkaline Hydrolysis of 2,4, Pentane-dione; Conductivity Method presented at the Fourteenth Annual Symposium in Chemistry held at the Indian Institute of Technology, Madras during March 4 – 5, 1989.
  20. Oxidation of Camphor by Phenyliodoso acetate presented at the Tenth Annual Symposium in Chemistry held at the Indian Institute of Technology, Madras during March 9 -10, 1985.
- **Hobbies:** Chess, reading, swimming, badminton, table tennis, bush walking.
- **Personal Habits:** I have never taken any drugs or smoked in my life. I am extremely hard working and persevering by nature with an enquiring mind and this enables me to fit easily into any group.

### Language Skills

- ❖ **Very fluent in English.** Had all education from primary level in English. My parents and grand parents spoke English fluently. As English is the medium of instruction at the University level in India, I have been lecturing in English and marking answer papers, records, lab reports thesis and dissertations written in English throughout my teaching career. Hence my English is excellent.
- ❖ Indian languages known to read, write and speak fluently are Malayalam, Tamil and Hindi.
- ❖ Indian languages known to understand and communicate are Kanada, Marati, Punjabi and several other languages.

### Refresher Courses Attended

- All India Refresher Course on Group Theory and Chemistry sponsored by the UGC held at Madras Christian College, Tambaram, Chennai, 600059 from 28<sup>th</sup> November to 17<sup>th</sup> December 1983.

- UGC Refresher Course for Postgraduate Teachers in Chemistry (Physical Organic Chemistry) conducted by The Department of Organic Chemistry, Division of Chemical Sciences, Indian Institute of Science, Bangalore, 560012 from 12<sup>th</sup> to 27<sup>th</sup> February 1991.
- UGC sponsored Refresher Course in Chemistry held at The School of Chemical Sciences, Mahatma Gandhi University, Kottayam, Kerala, 686560 from 9<sup>th</sup> February 5<sup>th</sup> March 1998.
- UGC Orientation Course (IT) for Postgraduate Teachers at the Academic Staff Training College, Trivandrum, Kerala from 7<sup>th</sup> October to 3<sup>rd</sup> November 2006.

### Co-Curricular Activities

Won numerous prizes in elocution, debating, essay writing, poetry writing etc. Won several prizes in indoor games like badminton, table tennis, chess and scrabble.

**At Balikamatom Girls High School, Thiruvalla:** Was the class leader in most of the classes and the school captain in the final year. Was a member of the school science club from 1970 –73 and the editor of the school magazine from 1971 to 73. Received the Science Talent award for the best innovative Science project from the whole district.

**At Mar Thoma College, Tiruvalla:** Was an active member of the Brains Trust, whose members are selected from the higher achievers within the college, from 1973 to 1978 and secretary of the Brains Trust from 1976 to 1978. Was a member of the Student Christian Movement from 73 –78 and the leader of SCM from 1977 to 1978. Was an active member of the National Service Scheme from 1976 to 1978. Attended several inter-collegiate camps and conferences under the auspices of the SCM and NSS.

Won the Proficiency Prize in English for scoring the highest marks among all the degree students – (BA, B.Sc. and B.Com.) of the college in 1977. Won the Proficiency Prizes in Mathematics in 1977 and Chemistry in 1978. Was the recipient of several prizes in English Elocution, Short Story Writing, Poetry Writing and Debating Competitions during 73- 78. Was a member of the college chess club and a member of the Women's Cricket team and badminton team from 1973 to 78.

**At Madras Christian College, Tambaram, Chennai:** Was the secretary of the Chemical Society from 1980 to 1981, the first ever female student to have held that office. Was the Mess secretary of the women's hostel during 1980-81. Represented the Residents Athletic Team which won the overall shield in the college sports meet in 1981. Won prizes in the scrabble, chess, badminton and table tennis competitions in 1980 and 1981. Won the first prize in Chemistry Quiz in 1980.

**As Faculty Member At Madras Christian College:** As the assistant warden of the women's hostel, from 1982 to 1984, helped the warden in the day to day administration of the hostel and managed the hostel alone for three months when the warden took leave due to illness. As the secretary of the women's staff and staff wives fellowship, from 1991 to 93 organized several programs for the campus families and children and also did social work in the neighboring slums. As the president of the Chemical Society, from 1985 to 1990 conducted several programs for the benefit of the students like organizing guest lectures, slide shows, career guidance programs etc. Conducted many inter class, intra department, and inter department competitions every year. Working in association with the Women's Studies group of the college, have done a lot of social work in the neighboring slums for the benefit of the poor women and children. As staff in charge of the Community Social Service, from 1981 to 1984 and 1996 to 1999 guided the students in social work like organizing cleaning programs, adult literacy classes, health and hygiene programs etc. directed towards the most needy sections of the society.

**At Indian Institute of Science, Bangalore:** Won the first prize in badminton singles, doubles, mixed doubles and table tennis doubles; second place in table tennis singles and mixed doubles and third place in swimming at the annual Gymkhana Tournament conducted for all the members of the institute. Was the only lady to complete the swimming Marathon 10,000 m in 1993. Was the only rated female chess player.

**In Australia:** As a member of the Canberra Olympic Swimming pool lap swimmers club completed 300 kilometers, swimming about 3 to 4 k every Sunday. Was a member of the ANU badminton club and ANU chess club. Was a member of the lap swimmers club of Melbourne City Baths and a member of Melbourne Chess Club.

## Referees

### Referees from Australia

1. Professor Adam J Bridgeman, Director of First Year Studies, School of Chemistry, Building F11, The University of Sydney, NSW, 2006, Australia. Phone: +61 2 9351 2731 Fax: +61 2 9351 3329 Email: [adam.bridgeman@sydney.edu.au](mailto:adam.bridgeman@sydney.edu.au) Web address: <http://sydney.edu.au/science/chemistry/research/bridgeman.html>
2. Professor Leo Radom, School of Chemistry University of Sydney, NSW 2006, Australia. Phone: 61-2-9351 2733 Fax 61-2-9351 3329 Email: [radom@chem.usyd.edu.au](mailto:radom@chem.usyd.edu.au) Web address: <http://www.chem.usyd.edu.au/research/radom.html>
3. Associate Professor Ronald J Clarke, First Year Lab Coordinator (2010 to 2014), School of Chemistry, The University of Sydney, NSW, 2006, Australia. Phone +61 2 9351 4406 Fax +61 2 9351 3329 Email: [ronald.clarke@sydney.edu.au](mailto:ronald.clarke@sydney.edu.au) Web address: <http://www.chem.usyd.edu.au/research/clarke.html>
4. Associate Professor Christopher D Ling, Second Year Lab Coordinator (2010 to 2013), School of Chemistry, The University of Sydney, NSW, 2006, Australia. Phone: +61 2 9351 4780 Fax: +61 2 9351 3329 Email: [chris.ling@sydney.edu.au](mailto:chris.ling@sydney.edu.au) Web address: [http://sydney.edu.au/science/chemistry/~ling\\_c/](http://sydney.edu.au/science/chemistry/~ling_c/)
5. Professor John Elix, Research School of Chemistry, Building 137, Australian National University, Canberra, ACT 0200, Australia. Phone 61 2 6125 2937 Fax 61 2 6125 0760 Email: [john.elix@anu.edu.au](mailto:john.elix@anu.edu.au)
6. Dr. Colin Rix, Adjunct Professor of Applied Chemistry, Faculty of Applied Science, Royal Melbourne Institute of Technology, Melbourne VIC 3001 Australia. Phone: +61 3 9925 2629 Fax: +61 3 9639 1321 Email: [colin.rix@rmit.edu.au](mailto:colin.rix@rmit.edu.au)
7. Dr. David Wilson, Lecturer, Department of Chemistry (Physical Sciences 3, Room 106), University of La Trobe, Melbourne, (Bundoora Campus) Victoria 3086, Australia. Tel: +61 3 9479 2553 Fax: +61 3 9479 1399 Email: [david.wilson@latrobe.edu.au](mailto:david.wilson@latrobe.edu.au) <http://www.latrobe.edu.au/chemistry/people/wilson.html>
8. Assoc. Prof. P.A.Tregloan, School of Chemistry, The University of Melbourne, Australia, 3010 Phone: +613 8344 7092 Fax: +613 9347 5180 [patreg@unimelb.edu.au](mailto:patreg@unimelb.edu.au)
9. Dr. David Chalmers, Lecturer Victorian College of Pharmacy, Monash University, 381 Royal Pde, Parkville, VIC 3053. Australia Phone: 9903 9110 Fax: +613 9903 9582 [David.Chalmers@vcp.monash.edu.au](mailto:David.Chalmers@vcp.monash.edu.au)

### Referees from India

1. **Dr. V J Philip, Retired Principal, Madras Christian College, Tambaram, Chennai, 600 059. Mobile +919500102306 E-mail: [vjphil@gmail.com](mailto:vjphil@gmail.com)**
2. Dr. Saraswathi Vishveshwara, Professor, Molecular Biophysics Unit, Indian Institute of Science, Bangalore, 560 012. E-mail [sv@mbu.iisc.ernet.in](mailto:sv@mbu.iisc.ernet.in)
3. Dr. P S Raghavan, Reader, Department of Chemistry, Madras Christian College, Tambaram, Chennai, 600 059 E-mail [ps\\_raghavan@rediffmail.com](mailto:ps_raghavan@rediffmail.com)

### Referees from US

1. Jayaraman Chandrasekhar, Gilead Sciences, 36 East Industrial Drive, Branford, CT 06405, Phone: 203 315 7412, Email: [jayaraman.chandrasekhar@gilead.com](mailto:jayaraman.chandrasekhar@gilead.com)
2. Professor Krishnan Raghavachari, Department of Chemistry, 800 E. Kirkwood Ave., Indiana University, Bloomington, IN 47405-7102, Phone: (812) 856-1766, Fax: (812) 855-8300 Email: [kraghava@indiana.edu](mailto:kraghava@indiana.edu) Web address: <http://raghavachari.chem.indiana.edu>
3. Professor H. Bernhard Schlegel, Department of Chemistry, Wayne State University, Detroit, Michigan, Phone (313)577-2562 E-Mail [hbs@chem.wayne.edu](mailto:hbs@chem.wayne.edu) Web address: <http://www.chem.wayne.edu/faculty/schlegel/>