

## Dr. G. Ramachandran



*Young Scientist (DST-SERB)*

*Department of Chemistry*

*School of Physical, Chemical & Applied Sciences*

**Date of Joining: 22/03/2016**

### *Academic*

S.No. Degree	Specialization	University / Institution	Year of Completion
1	Ph.D.	Theoretical/ Computational Chemistry	IIT-Kanpur 2007
2	M.Sc.	Chemistry	Kanchi Mamuniver Centre for Postgraduate studies (Affiliated to Pondicherry University) 1999
3	B.Sc.	Chemistry	Tagore Arts Collage (Affiliated to Pondicherry University) 1997

*Total Experience:* 2007 to present (2016)  
9 years

### *Area of Specialization:*

Theoretical and Computational Chemistry.

### *Research Interest:*

My present research interest focused in understanding the function of biomolecules by applying different theoretical methods. Future interest also involves in studying the non-covalent interaction between the molecules, reaction mechanism, structure based drug design, structural properties of molecules.

### *Postdoctoral Research Experience:*

1. Postdoctoral Research Scholar. Institute of Organic Chemistry and Biochemistry, AS, Prague, Czech Republic, May 2012 – Dec. 2015. **Adviser: Prof. Pavel Hobza**
2. Postdoctoral Research scholar. University of Nevada, Reno, U. S. A., July 2008 – July 2011. **Adviser: David M. Leitner.**
3. Postdoctoral scholar. University of Nottingham, Nottingham, U. K., 2007-2008. **Adviser: Prof. Jonathan D. Hirst.**

*Publications (list of selected publications):*

1. Hari Krishnan, Ramachandran G., Ramaraj, R. C. “Controlled, Sequential approach to Synthesize Sterogenic Methanes via In-situ Generated Reactive Intermediates” *ChemistrySelect*, 2016, 1, 3022-3027.
2. Sunil R., Praveen S., Ranjeet K., Ashish T. K., Jiří Hostaš, Ramachandran G., Pavel Hobza “Experimental and Theoretical Study on Assessing the Conformational Stability of Polymethylene Bridged Heteroaromatic Dimers: A Case of Unprecedented Folding” *Crystal Growth and Design*, 2016, 16, 1176-1180.
3. Susanta Halder, Ramachandran G., Pavel Hobza “A comparison of *ab-initio* Quantum- Mechanical and Experimental Do Binding Energies for Eleven H-Bonded and Eleven Dispersion-Bound Complexes” , *PCCP*, 2015, 17, 26645-26652.
4. Jiří Hostaš, Dávid Jakubec, Roman A. Laskowski, Ramachandran G., Jan Řezáč, Jiří Vondrášek, Pavel Hobza “Representative Amino Acid Side Chain Interactions in Protein - DNA complexes. A Comparison of Highly Accurate Correlated *ab initio* Quantum Mechanical Calculations and Efficient Approaches for Applications to Large Systems”, *J. Chem. Theory Comput.* 2015, 11, 4086-4092.
5. Ashish T.K., Priyanka S., Ved P. S. Praveen. S., Pankaj S., Ramachandran G., Hobza P., “Selective induced polarization through electron transfer in non-polar substrates”, *New Journal of Chemistry*, 2014, 38, 4885-4892.
6. Johnson K. A., Ramachandran G., Leitner D. M., "Communication Maps: Exploring Energy Transport Through Proteins and Water" *Israel Journal of Chemistry*, 2014, 54, 1065 - 1073.
7. Ramachandran G. “Normal Modes and Duschinsky Mixing of Ground and Excited State Vibrations of the Green Fluorescent Protein Chromophore” *Chem. Phys. Lett.* 2013, 587, 61-67.
8. Yao X., Ramachandran G., Leitner D. M.,”The dielectric response to photoexcitation of GFP: A molecular dynamics study” *Chem. Phys. Lett.* 2013, 564, 78-82.
9. Yao X., Ramachandran G., Leitner D. M.,”Analysis of water and hydrogen bond dynamics at the surface of antifreeze protein” *J. At. Mol. and Optical Phys.* 2012, 2012, Article ID 125071.
10. Ramachandran G., Leitner D. M.,”Dielectric response and vibrational energy relaxation in photoactive yellow protein: a molecular dynamics simulation study” *Chem. Phys. Lett.* 2011, 516, 102-105.
11. Ramachandran G., ”Vibrational Spectra of Cyclooctatetraene alkali metal complexes [C<sub>8</sub>H<sub>8</sub>M<sub>2</sub> (M= Na,K)]” *Vibrational Spectroscopy*, 2011, 57, 288-293.
12. Ramachandran G., Johnson K. A., Leitner D. M., ”Communication maps computed for homodimeric hemoglobin: Computational study of water mediated energy transport in proteins” *J. Chem. Phys.* 2011, 135, 065103. (Editor's choice 2011, also selected as one among the outstanding articles to celebrate 80th anniversary of The Journal of Chemical Physics).

13. Ramachandran G., Yao X., Leitner D. M., "Dynamics of water confined in proteins: A molecular dynamics simulation study of interfacial waters in a dimeric Hemoglobin" J. Phys. Chem. B 2010, 114, 16989.
14. Diedrich A. S., Ozgur B., Stefen F., Benjamin P.B., Ramachandran G., Gerard W. S., Leitner D. M., and Martina H. "Rattling in the cage: Ions as probes of sub-picosecond water network dynamics". J. Am. Chem. Soc. 2009, 131, 18512.
15. Ramachandran G., Manogaran S., "Vibrational spectra of triamantane  $X_{18}H_{24}$ , isotetramantane  $X_{22}H_{28}$  and cyclohexamantane  $X_{26}H_{30}$  ( $X = C, Si, Ge, Sn$ ): A theoretical study". J. Mol. Struct. Theochem, 2007, 816, 31.
16. Ramachandran G., Manogaran S., "Vibrational spectra of adamantanes  $X_{10}H_{16}$  and diamantanes  $X_{14}H_{20}$  ( $X=C, Si, Ge, Sn$ ): A theoretical study". J. Mol. Struct. Theochem, 2006, 766, 125.
17. Ramachandran G., Manogaran S., "Vibrational Spectra of  $C_{20}H_{20}$ : A theoretical study". J. Mol. Struct. Theochem, 2005, 730, 171.
18. Ramachandran G., Manogaran S., "Vibrational Spectra of cubane and azacubane: a theoretical study". J. Mol. Struct. Theochem, 2005, 719, 7.
19. Tinabaye A., Ramachandran, G., Ganesan, T., "Antifungal Activity of usnic acid isolated from usnea Albopunctuata". Geobios, 2001, 28, 167.

#### **Seminars/Conferences/Workshops Participated:**

- 1, "10<sup>th</sup> European workshop in Drug Design", May 17-22, 2015, Siena, Italy.
2. "The 14<sup>th</sup> Theoretical Chemistry Symposium", Dec 18-21, 2014, CSIR-NCL, Pune, India.
3. Workshop on "Recent progress in adiabatic and non-adiabatic methods in quantum dynamics", CECAM, EPFL, Lausanne, Switzerland, May 12-15, 2014. Poster: "Normal Modes and Duschinsky Mixing of Ground and Excited State Vibrations of the Green Fluorescent Protein Chromophore".
4. Workshop on Molecular Kinetics, Sept. 2-5, 2013, Berlin. Poster: "In-Silico Drug Design for Carbonic Anhydrase Protein Enzymes".
5. CRC International Symposium in Strasbourg: Chemical Theory for Complex System, Mar. 7-8, 2013, ISIS, University of Strasbourg, France.
6. 241<sup>st</sup> ACS National Meeting, Anaheim, California, U. S. A., 27-31 March 2011. Poster: "Dynamics of water clusters confined in proteins and their role in energy transport: A molecular dynamics simulation study of interfacial waters in a dimeric hemoglobin".
7. 28<sup>th</sup> Graduate Student Meeting University of Manchester, 16<sup>th</sup> April 2008.
8. The 17<sup>th</sup> Annual Northern Universities Meeting on Chemical Physics (ANUMOCP), Leeds, U.K. 11<sup>th</sup> July, 2007.

9. Trends in Theoretical Chemistry, Bhabha Atomic Research Center, December 9-12, 2004. Poster: “*Vibrational spectra of Cubane and Azacubane: A theoretical study*”.

10. National Symposium: Chemical Research Society of India, IIT Kanpur, February 6-8, 2004. Poster: “*Vibrational Spectra of Acetophenone and acetylpridines: A theoretical study*”.

11. Trends in theoretical Chemistry, IACS, Calcutta, January, 2003. Poster “*Vibrational spectra of Icosahedral symmetric molecules: B<sub>12</sub>H<sub>12</sub><sup>2-</sup>, C<sub>20</sub>H<sub>20</sub> and C<sub>60</sub>*”.

12. National Symposium on Radiation and Photochemistry (NSRP-2003), IIT, Kanpur, India, 3-5 March 2003. Poster “*Vibrational spectra of adamantane and diamantine*”.

#### *Invited Talks (in last 3 years):*

1. Vellore Institute of Technology- “Binding Capabilities of Nido-heteroboranes: Effect of Total Charge” 13<sup>th</sup> Jan. 2016, Vellore, India.
2. Pondicherry University – “Computational Studies on Small and Macromolecules” 3<sup>rd</sup> March, 2016, Puducherry, India.
3. SRM University – “Computational Studies on Biomolecules” May, 2016, Chennai, India.

#### *Honours / Awards:*

- 1) Qualified in Graduate Aptitude Test in Engineering (GATE), India-2000
- 2) **Royal Society Fellowship** 2007-2008.
- 3) Awarded as **the DST-SERB Young Scientist** in 2016.

#### **Projects Undertaken: Ongoing/completed Projects:**

“*Classical and quantum mechanical approaches to study the process of polymerization in HIV-1 reverse transcriptase*” Sponsor: Department of Science and Technology, Govt. of India. Duration: 2016 to 2019. Role: PI

M.Sc. Project: 1 (on going)

#### *Contact Details*

##### **Present Address:**

Dr. G. Ramachandran,  
Young Scientist (DST-SERB),  
Department of Chemistry,  
Pondicherry University, Kalapet,  
Puducherry - 605 014, India.

**Telephone No:** 0413-2654 708

**Mobile No:** +91-9677740254 & +91-8903710766

**Email:** [gtrama@gmail.com](mailto:gtrama@gmail.com)