

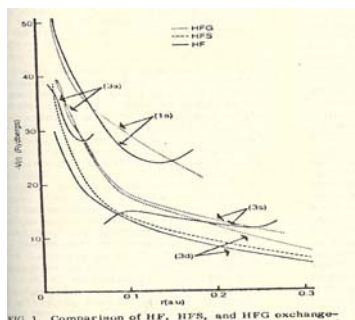
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Biographical:

- Born 1942 Elanthur, Kerala
- Masters in Chemistry 1965 University of Kerala
- PhD 1972 Indian Institute of Technology Kanpur
- Royal Society (London) Bursar 1972-1974
University of Oxford, England
- National Research Council of Canada Fellow,
1974-1977 McGill University, Montreal, Canada
- Assistant Professor of Chemistry, 1977-1986
IIT Madras
- Professor of Chemistry 1986- present, IIT Madras
- Alexander von Humboldt Fellow, Germany
1982-83, 1987, 1988 University of Hannover,
1991 Technische Hochschule, Darmstadt
- Married 1974 to Dr. Kamala Gopinathan PhD;
son: Dr. Ajay Gopinathan PhD, University of
California, USA.

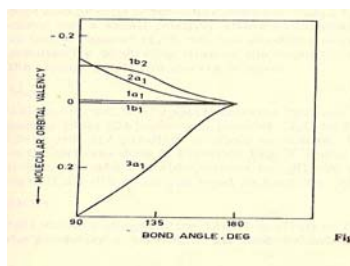
Highlights of Research Accomplishments:

The two major areas of research have been:
 (a) Quantum Chemistry and
 (b) Nonlinear dynamics in Chemistry and Biology.



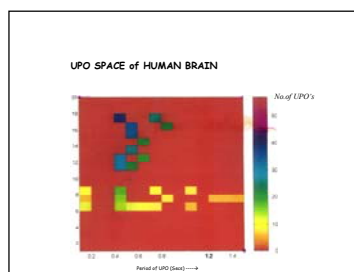
HFG Potential (Phys. Rev. A. 1977)

In the 1970's and 1980's developed accurate atomic and molecular potential fields from *ab initio* principles. Demonstrated its successful use in calculations of various atomic and molecular structure properties. These developments were the forerunner of the present day Density Functional Theory widely used by Chemists and Physicists in molecular property computations. Relativistic and electron correlation effects were successfully incorporated into the formalism in later years.



MO valencies in H₂O (J. Amer. Chem. Soc. 1988)

In the 1980's a quantum mechanical definition of **chemical valency** was introduced and developed in further work. This concept enables the quantitative rationalization of electronic and geometric structure of molecules. The concept of valency was generalized for molecular orbitals. The preferred course of chemical reactions could be predicted using this concept of valency.

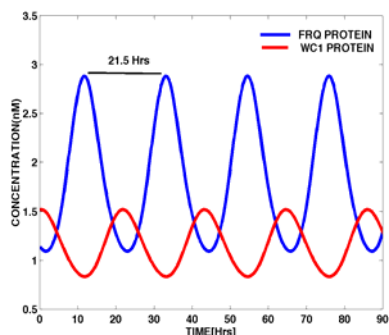


UPO spectrum of Human brain for various states of consciousness
 Adapted from Nonlinear Dynamics and Brain Functioning",
 Nova Science Publishers 2000

In recent years our attention is focused on experimental and modeling studies of **nonlinear dynamical phenomena** in chemistry, biochemistry and physiology. Based on rigorous analysis of extensive experimental data on human ECG and EEG, we have established the "chaotic" nature of the human cardiac and brain systems.

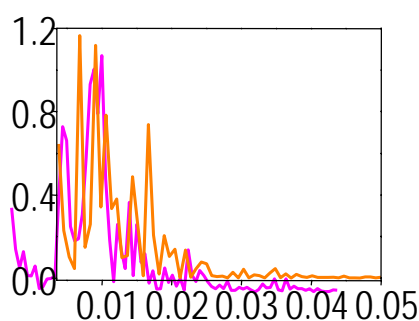
The concept of Unstable Periodic Orbits (UPO) spectrum has been introduced to analyse the dynamics of such systems. It is shown that the UPO spectrum clearly distinguishes several *cardiac pathologies* and *states of consciousness of the brain*

We have shown recently that complex biochemical reaction networks can be quantitatively modeled efficiently using **Dealy Differential Equations**. Many parts of the network can be represented by time delays. Our technique has been applied to model *circadian rhythms* and *cell division cycles*.



Simulated Circadian Oscillation in Neurospora Crassa, J. Theor. Biol. 2004

A simple two-variable nonlinear delay equation model can describe quantitatively the circadian protein oscillations in the fungus *Neurospora crassa*. We have also found that external “noise” can generate and amplify circadian oscillations. This is an instance of the occurrence of “stochastic resonance” phenomenon in a biological rhythm.



Experimental (-----) and simulated (-----) oscillations of CO₂ over melting ice. Phys. Rev. Lett. 2004

In our latest work, we have applied nonlinear dynamical model to explain the **oscillations of CO₂ gas** over melting ice, observed in our laboratories. This observation and its theory are expected to have deep geological and environmental implications.

Selected Publications:

(Total ~ 75 in international journals)

1. Concentration of CO₂ over melting ice oscillates, S Usharani, J Srividhya, **M S Gopinathan** & T Pradeep, *Phys. Rev. Letts.* 93, No.4 , 2004
2. A two variable dealy model for the circadian rhythm of *Neurospora crassa*, K Sriram & **M S Gopinathan**, *J. Theoret.Biol.* , in press, 2004
3. The role of time delay and noise in chemical and biological rhythms, **M S Gopinathan**, Invited article in Special Issue of *Proc. Ind. Nat. Sci.Acad.*, in press, 2004
4. Oscillatory mass transfer across liquid membrane, J Srividhya & **M S Gopinathan** *J. Phys. Chem. B.*, 107,1438, 2003
5. Nonlinear analysis of continuous ECG during sleep I. Reconstruction, J. Fell, K. Mann, J. Roschke & **M S Gopinathan**, *Biol. Cybern.* 82, 477 ,2000
6. The spectrum of unstable periodic orbits of the human brain, R B Govindan, K. Narayanan, **M S Gopinathan**, N. Pradhan, R Sreenivasan and P Dwivedi, in :*Nonlinear Dynamics and Brain Functioning*”, Nova Science Publishers, NY, 345 , 2000
7. Chaos in Chemistry and Biology, **M S Gopinathan**, in “Advances in Physical Chemistry”, ed. T Pradeep, Allied Publishers, New Delhi, 1999
8. Unstable periodic orbits in human cardiac rhythm, K Narayanan, R B Govindan & **M S Gopinathan**, *Phys. Rev.E.*, 57, 4594, 1998

9. *Dynamics from time series: Iterative maps in correlation space*, **M S Gopinathan**, *Proc. Ind. Acad. Sci. (Chem. Sci.)*, 106, 479 (1994)
10. *The quantum chemistry of valency*, **M S Gopinathan**, *Proc. Ind. Acad. Sci. (Chem. Sci.)* 96, 167, 1986
11. *Valency correlation diagrams*, Prabha Siddarth & **M S Gopinathan**, *J. Amer. Chem. Soc.*, 110, 96, 1988
12. *The quantum chemistry of valency*, **M S Gopinathan**, *Proc. Ind. Acad. Sci. (Chem. Sci.)*, 96, 167, 1986
13. *Relativistic Xi method for atoms*, V Selvaraj and M S Gopinathan, *Phys. Rev. A*, 29, 3007, 1984
14. *Improved approximate representation of the Hartree-Fock potential in atoms*, **M S Gopinathan** *Phys. Rev. A* **15**, 2135, 1977
15. *The Fermi hole and the exchange parameter in X_α theory*, **M S Gopinathan**, M A Whitehead & R Bogdanovic, *Phys. Rev. A* 14, 1, 1976

Ph. D. Scholars Guided:

- Ravimohan, C.
- Vaidehi, N
- Selvaraj, V
- Vijayakumar, M
- Prabha Siddarth
- Narayanan, K
- Govindan, B
- Moni, M.S.
- Baby, C.
- Sriram, K
- Srividhya, J. (on going)

Teaching & Computing Innovations:

- Developed and taught several courses at IIT Madras for B Tech Freshers, Masters and Ph.D. Scholars.
- Courses developed as Computer Assisted “*live course material*”, using software like MATLAB, MATHEMATICA, *SCIENTIFIC WORKPLACE*. Class Instruction thus becomes participatory and creative rather than passive.
- Introduced at IIT a course on “*Methods in Computational Chemistry*” – a popular course for Masters and PhD scholars in Chemistry, Physics and Mathematics.
- Developed and supervised development of extensive codes for atomic and molecular quantum mechanical as well as nonlinear dynamical computations – in FORTRAN, C, MATHEMATICA & MATLAB

- Pioneered the use of Internet and Online courses in Classroom Instructions.
- Developed a Tutorial Package on Introduction to Nonlinear Dynamics in MATLAB for distribution to various universities and institutions under the Educational Technology Cell of IIT Madras.

Book

Group Theory in Chemistry
Vishal Publishers, New Delhi, 1985
(A textbook at several Universities in India, Reprinted every year)

Distinctions/Awards

- Fellow Indian National Science Academy, New Delhi
- Fellow Indian Academy of Science, Bangalore
- Fellow Sigma Chi of North America
- Fellow Alexander von Humboldt Foundation Germany
- Bursar Royal Society London
- National Merit Scholarship of India
- Linus Pauling Lecture Award 2003 Mahatma Gandhi University, Kottayam
- Invited Speaker/Chairman at various National and International Conferences and Universities.

Cultural Interests:



Poetry writing;
 Dramatics - writing, acting

As Gandhi in "The Trial of Gandhi"
at IIT Madras, 1997