



**MOLECULAR MODELLING, SIMULATION AND  
ENGINEERING GROUP**  
ESCOLA DE QUÍMICA, UNIVERSIDADE FEDERAL DO  
RIO DE JANEIRO

Rio de Janeiro, June 15<sup>th</sup>, 2000

To

Prof. V. Sitaramam,  
Department of Biotechnology  
University Of Pune  
Pune 41107  
India

Dear Prof. Sitaramam

I would like to visit your laboratory for a period of 6-8 weeks in this year. I enclose my latest CV. I would appreciate if you could forward this to an appropriate government agency to arrange an invitation. I will accept any government invitation for me to visit India and work with you.

You were suggesting the possibility of taking this up with department of Biotechnology. I would like that. The work we are doing and plan to complete to some measure now of importance in polymer physics. As a consultant to Petrobras, the Brazilian equivalent of the Indian ONGC, this work has bearing on all aspects of polymers. In case of biopolymers, I would expect it to be path breaking. Since the combined work, we already published is so well received, I have no hesitation in thinking that further work would be very important indeed.

I shall look forward to visiting you and would be obliged for whatever processing you would need to do to arrange a visit from Rio de Janeiro to Pune and back.

Thanking you,  
Yours sincerely,

*K. Rajagopal*

K. Rajagopal.  
Professor Titular .

**Plan of work for the visit of Dr. Rajagopal in 2000. Collaborative work between Prof. V.Sitaramam (Biotechnology Dept.) Dr. A.D.Gangal (Physics Dept.) and Prof. Rajgopal (UFRJ, Rio de Janeiro, Brazil)**

Dr Rajgopal and, I, Prof. V. Sitaramam are involved in a alternative description of biopolymers in which we develop the idea that the protein is not a diad of the chain and the solvent but a triad of the polymer, the solvent and space (voids), which we published in a J. Theoret. Biol. paper(enclosed). A great deal of experimental work is on the way from my laboratory at the moment drawing heavily from this theoretical work.

Dr. Rajagopal forms part of a team we have now along with theoretical physicists from our University, particularly Dr. A.D.Gangal and we have a programme for the minimal description of biopolymers and their functions from a polymer physics point of view. A project was supported by DBT earlier in this regard a paper has been published for void formation in 2-D solutions of disks. One paper has already appeared in Physica A and others are under communication from this group.

Dr. Rajagopal would be coming for formulating a specific research plan with us for our ongoing work, which has deep implications in protein engineering and biopolymers. He would

1. Do research and act on an existing specific plan: I also enclose a specific action plan we have formulated for our theoretical work in this visit as enclosed.
2. Help in writing some manuscripts in which he has to contribute statistical mechanics and thermodynamics of polymers
3. Dr. Rajagopal would also be involved in finalizing research proposals which we already submitted to ISRO, and
4. He would also interact in teaching.

PTO

### What to do with voids in Biopolymers: *a specific action plan*

We have proposed for the first time that biopolymers consist of not merely the polymer and solvent but also the space intrinsic to the polymer, nontrivially termed voids. The thermodynamics has been solved, measurement methods have been developed and the ramifications now need to be explored virtually in all areas of biology in terms of polymer physics. Below is a plan of action for work envisaged between three of us.

The problem is in three parts :

1	<b><i>How to generate and measure voids</i></b>	1a. Spherical shell interactions (Steele, 1964 J. Chem.Phys.)Most Urgent!! 1b. Linked phantom chain dynamics 1c. For long chains, rattle & shuffle methods 1d. Algorithms to measure voids in silico in biopolymers 1e. 3-D simulations relative effects of prolate and oblate ellipsoids
2	<b><i>Characteristics and thermodynamics of voids</i></b>	2a. Local composition. 2b. Lateral diffusion 2c. Connectivity of pores...forest fire models 2c. Tortuosity, permeability and porosity
3	<b><i>How to use voids in mechanisms</i></b>	3a. Cavity factors in solvation 3b. Historical origins of voids: multicomponent adsorption ---vacancy solution theory. 3c. biology 3d. Active applications: <ul style="list-style-type: none"> <li>i. land-filling, chemical dump linings</li> <li>ii. water purification (ground water)</li> </ul> 3e. Developmental stages of applications <ul style="list-style-type: none"> <li>i. Pervaporation __ alcohol /H2O mixtures and alcohol separation</li> <li>ii. Oil sludge/ sea water separation</li> </ul> 3f. Research <ul style="list-style-type: none"> <li>i. microelectronics: deposition of magnetic media and catalyst media(metals) in pores of fixed dimensions and derivatives.</li> </ul>