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### **Employment History**

Jul 2001 – present : **Deputy Executive Director**, , Bioinformatics Institute, Singapore,  
Jul 1996 – Jun 2001 : **Assistant Director of Research**, Cavendish Laboratory, University of Cambridge,  
Sep 1997 – Jun 2001 : **Teaching Fellow & Director of Studies**, Jesus College, Cambridge  
Apr 1994 - Jun 1996 : **Postdoctoral Research Associate**, , Cavendish Laboratory, University of Cambridge,  
Sep 1993 - Mar 1994 : **Visiting Research Fellow**, School of Physics, Georgia Tech, Atlanta, Georgia, USA,  
Sep 1991 - Aug 1993 : **Postdoctoral Research Associate**, , Cavendish Laboratory, University of Cambridge,  
Sep 1987 - Aug 1991 : **Director's Research Assistant**, , School of Physics, Georgia Tech, Atlanta, Georgia, USA,  
Jun 1986 - Aug 1987 : **Lecturer and Head of Physics**, , Prime College, Kuala Lumpur, Malaysia,  
Jan 1984 - May 1986 : **Lecturer in Physics**, , Damansara College, Kuala Lumpur, Malaysia,  
Jun 1981 - Dec 1983 : **Physics Instructor**, , University of Malaya, Kuala Lumpur, Malaysia

### **Research Interests**

I have published 36 peer reviewed papers in computational physics and chemistry. In the past, my research has been focused on developing techniques based on density functional theory and Quantum Monte Carlo on massively parallel computers to investigate the electronic structure and properties of real materials. I am currently leading a research group focused on modeling Signal Transduction. The group consists of a postdoc, a research associate and three PhD graduate students. My current research is focused on developing and applying theoretical concepts, mathematical methods and computational techniques, to understanding the principles and mechanisms responsible for control and regulation of the cellular process such as gene regulation and signal transduction. We have initiated a number of projects involving collaborations with academia and the pharmaceutical industry:

- **Developing Mathematical & Computational techniques for Stochastic Chemical Kinetics:** (With Postdoctoral associate Dr. Chiam Keng Hwee and research associates Mr. Vipul Bhargava and Mr. Li Bin). A crucial component of our project is the ability to quantitatively replicate the chemical kinetics occurring in mesoscopic systems such as that within the cell. We are developing mathematical and computational techniques to

incorporate stochasticity into our pathway models, to quantify the effects of noise on system-level properties.

- **Identifying Intestinal Stem Cells and Imaging Epithelial Migration:** (Flagship project within the Singapore-MIT Alliance in collaboration with Prof. Paul Matsudaira, WI and Prof. Birgit Lane at the Center for Molecular Medicine) - To work within the SMA Computational and Systems Biology Initiative to pursue the following aims: (1) to use a combination of microarray and bioinformatics to identify specific stem cell markers which will facilitate their in vivo study via high-resolution real-time imaging of live tissues; (2) to identify the factors that regulate aspects of the behavior of stem cells such as the process of asymmetric division and differentiation etc. ultimately leading to a deeper understanding of the nature of “stemness”; (3) to develop quantitative models to explore how a gradient of Wnt morphogens along the crypt-villus axis in the small intestine can regulate proliferation and differentiation status as epithelial cells migrate from the crypt to the tip of the villus; (4) to elucidate the mechanism of epithelial cell migration in the epithelium of the small intestine of the Zebrafish using real-time high-resolution in vivo imaging of live tissue. To this end we will work closely with our experimental collaborators at IMCB, NUS/DBS, CMM and NUS/BioEng to obtain and analyze the data they collect to build quantitative models. The data obtained, together with all publicly available data on adult stem cells, will be collected and curated in a Stem Cell KnowledgeBase that will be available to the whole community.
- **Control and regulation of p53: (a) Imaging and Modeling of the p53-Hdm2 Feedback Loop: Role of Activator-Inhibitor Motifs in regulation of cellular processes; (b) A Systems Biology Approach Elucidating the Role of the P38 MAPK Pathway and its Interactions with the p53 Mediated Cell Cycle Control Checkpoints in Tumor Suppression.** (With Ph.D. student Mr. Mark Phong of Eli Lilly Systems Biology Singapore, Dr. Christopher Taylor of Lilly System Biology Singapore, Dr. Xiang Yi at Eli Lilly USA and Prof. Sir David Lane’s Group at IMCB, Singapore.). (a) Recently, Lahav et. al. (Nature Genetics, 36, 147, 2004) reported results of damped oscillations of p53/mdm2 proteins in individual living cells when subject to stress. They found that p53 was expressed in a series of discrete pulses after DNA damage. Their main conclusion is that the p53-MDM2 feedback loop generates a “digital” clock that releases well-timed quanta of p53 proteins until damage is repaired or the cell dies. Our aim, through a combination of experiment and quantitative modeling, is to verify that these observations are indeed correct and to elucidate the mechanism that gives rise to the “digital pulses”. (b) To study the role of p38 MAPK as a tumor suppressor we plan to: 1. To collect and annotate data related to developing a comprehensive map of the p38 MAPK pathway and its role in p53 mediated cell cycle control for the purposes of building a computational model that accurately describes the signal transduction process; 2. To formulate an appropriate mathematical and computational framework describing the simplified network topology of the p38 MAPK pathway and the p53 cell cycle response to genotoxic shock and DNA damage; 3. To validate the accuracy and veracity of the quantitative model through bench biology experiments on model cell lines enhancing the model iteratively; 4. Expansion from single cell model to cell population model.

- Modeling Differential Gene Expression: A Systems Biology Approach to Elucidate the Frequency Decoding of GnRH Signals that Governs the Differential Expression of Mammalian Gonadotropin Subunit Genes.** (With AGS Scholar Stefan Lim and Dr. Philippa Melmlud (DBS, NUS)): Luteinizing and follicle-stimulating hormones (LH and FSH) are gonadotropic hormones synthesized in the pituitary gonadotropes. They share a common  $\alpha$ -subunit but contain a unique  $\beta$ -subunit that confers physiological specificity. LH and FSH directly stimulate gonadal growth and steroidogenesis, therefore regulation of the precise levels of each hormone is critical to correct reproductive functioning. The hypothalamic GnRH regulates both hormones, and variations in its pulse frequency are associated with the differential effects on each of the three subunits. The mechanism by which gonadotropes decode varying gonadotropin-releasing hormone (GnRH) pulse frequencies and translate them into differential gene expression is unknown. It is the goal of this project to resolve this issue through an integrative approach involving a fusion of biological, genetic, computational and mathematical techniques. Understanding the molecular mechanisms that control gonadotropin biosynthesis holds great potential for the clinical treatment of a variety of reproductive disorders. The knowledge gained in the resolution of this problem will also contribute to a deeper conceptual understanding of the mechanisms governing differential expression of genes in general, which is the cornerstone of developmental biology.
- Modeling Mechanotransduction - A Systems Biology Approach to Elucidate the Role of Adhaerens Junctions and Tight Junctions as Mechanotransducers in Regulating Cell Proliferation.** (With AGS Scholar Lim Tong Seng, Dr. Lim Chwee Teck (BioEng, NUS), Prof. Paul Matsudaira (Biology and BioEng, MIT) and Prof. B. Lane, Center for Molecular Medicine, Singapore) – Mechanotransduction or the translation of mechanical forces into biochemical signals; plays an important role in the regulation of cellular activities. How cells sense external forces and integrate these forces at the molecular level to produce coordinated responses is an open question. In particular, the mechanism by which mechanical stimuli regulate cell proliferation is a subject of great controversy and a resolution to this issue has wider implications both for the fundamental understanding of cell biology and within a clinical context. To this end, we are investigating specific classes of proteins found in tight junctions and adhaerens junctions, which are specialized cell-cell contacts that play an important role in regulating cellular activities. This project aims to test the hypothesis that specific members of the tight and adhaerens junction proteins act as mechanotransducers for regulating cell proliferation when quiescent epithelial cells in culture are subjected to mechanical stimuli.

### Academic Qualifications

**Ph.D. Physics**, December 1991, Georgia Institute of Technology,

Thesis: *Systems of Coupled Classical and Quantum Degrees of Freedom*

**M.S. Physics**, December 1989, Georgia Institute of Technology

**M.Sc. in High Energy Physics**, August 1984, University of Malaya,

Thesis: *Exact Calculation of the Quark-Photon Vertex*

**B.Sc.Ed. Physics/Mathematics/Education**, August 1981, University of Malaya

## Teaching Experience

**At the Bioinformatics Institute, Singapore:** Supervising four AGS PhD students in Systems Biology and Bioinformatics. I lecture graduate courses in Computational Biology, Molecular Modeling and Mathematical/Systems Biology and Systems Biology of Cancer/Stem Cells. I also supervise MSc/PhD research projects in all aspects of bioinformatics and computational/systems biology. I lead study sessions on mathematical methods applied to biological problems. Details of my achievements in setting up and directing a graduate program in bioinformatics/computational biology will be provided on request.

**At the University of Cambridge, UK:** I supervised a M. Phil. student (Churchill Scholar, awarded degree in December 1999), and Co-supervised seven Ph.D. students at the Cavendish Laboratory (1992-2001) and three PhD students at Imperial College, London. I lectured a Part II (3rd year) undergraduate physics course (Theoretical Physics I/II), and Part III (4th year) course, "Supercomputing in Physics", as well as supervised Literature Reviews and Part III projects, at the Cavendish Laboratory. I gave postgraduate lectures on high performance computing, biological physics and electronic structure theory at the Cavendish. I supervised Physics undergraduates in Part II (3rd year) Quantum Mechanics, Solid State Physics, Thermal Physics, Systems, Part III (4th year) Solid State Physics, Part IB Advanced Physics and Mathematics for IA and IB (Natural Science), as well as Part II Literature Reviews and Part III Projects (1996-2001).

**At the Georgia Institute of Technology, USA:** Lectured freshman and sophomore Engineering Physics courses at Georgia Tech. Duties involved presenting lectures and grading (1989-1991).

**At the University of Malaya, Malaysia:** Physics instructor at the University of Malaya. Duties involved supervising and grading third year undergraduate laboratory courses (1981-1983).

**At Damansara/Prime Colleges, Malaysia:** Prepared students in Physics, Pure and Applied Mathematics, for the A-level examinations (Oxbridge Examination Boards), at Prime College, and Damansara College, Malaysia (1984-1987) and lectured freshmen students in the American Program.

## Management Responsibilities

### In Singapore:

**At the Bioinformatics Institute:** I set up the Institute from scratch in July 2001. The mission of the BII encompasses research in bioinformatics and computational biology, post-graduate education, IT and application support for the biomedical user community in Singapore and cyber-infrastructure development at the national level. The BII serves as the central national resource for biomedical computing for the biomedical research community. Within the BII, my responsibilities include setting up and overseeing the management, research, biomedical computing support and post-graduate education activities of the Institute (currently 120 staff members and 39 graduate students). I am also the program driver for the P53 and Stem Cell Initiative that links experimental and quantitative modeling researchers within the Biopolis to address key biomedical questions in cancer and stem cell biology and to coordinate the building of a Web based knowledgebase to advance R&D in these areas.

**Cross Institution responsibilities:** Chairman of the Joint Management Committee overseeing the BII-NUS Postgraduate Program in Bioinformatics. Planned and implemented a graduate program in Bioinformatics involving 2 years of course work and academic and industrial attachment. I currently head the Academic Program at the BII.

**Research Council Responsibilities:** Chairman of the IT Steering Committee for the Biomedical Research Council and Co-Chair of the One-north IT steering Committee responsible for planning, implementing and managing the outsourced cyber-infrastructure and services for the new science park, the Biopolis (Project SELECT). The Biopolis ([www.one-north.com](http://www.one-north.com)) is a physical co-location of public and private research institutes and biotech companies that will leverage on each other to advance biomedical research and development and exploit the results of the research for wealth creation. The Project Team responsible for formulating, managing the tender process and the implementation of infrastructure and services is located within the BII and I chair the weekly coordination meetings.

The computing cyber-infrastructure is planned so as to help address the deluge of data (genomic and clinical) that are emerging from high throughput experiments, and meet the evolving needs of the biomedical user community. The BII will be the central resource (computing and expertise) for biomedical computing for the biomedical research community.

**National Cyberinfrastructure responsibilities:** I am a member of the Steering Committee for the Singapore National Grid Initiative whose goal is to aggregate national computing resources to effectively and efficiently address the needs of academia, industry and the medical community. To build up the expertise to accomplish this challenging task, I am leading the Singapore BioMed Grid (BMG) Project responsible for integrating cyber-infrastructure within Singapore (and in collaboration with similar Grid projects in the US and Europe especially the UK e-Science initiative). The main focus is to develop and implement grid-based middleware and application software of interest to the biomedical community to advance research and development in the public and private sector. We work very closely with companies such as Intel Sun and HP as well as the US national supercomputing centers (NCSA, PNNL and SDSC) to share expertise in developing grid computing for the biomedical user community. We are founding members of international collaborations in grid computing such as the PRAGMA Consortium and the GELATO Federation.

#### **At the University of Cambridge, United Kingdom:**

**Cross-Department Responsibilities:** Coordinator and member of management committee of the Cambridge High Performance Computing Facility (1994-2001). My responsibilities included management of the day to day operation of the University of Cambridge High-Performance Computing Facility. This includes providing technical advice to the user community within the University on all aspects of high performance computing. I am also involved in the enhancement of supercomputing resources by preparing grant applications to funding bodies.

**Cavendish Laboratory, University of Cambridge:** Part III Physics Examiner for the 1998/1999 and 1999/2000 academic years. Working with three other examiners, I set questions for the General Paper and mark it. I also am involved in checking and preparing the Special and Minor Topics papers.

**Research Council Responsibilities:** Member of the EPSRC "Computational Partial Differential Equations" Panel (1998-2001). I refereed grant applications for EPSRC and HEFCE/JREI.

**Jesus College:** Elected member of Jesus College Governing Council. The college council meets every fortnight and is charged with overseeing all aspects of college government including educational, financial, social matters and the supervision of full-time college officers. Elected to the Mastership Committee (April 2000), to help select the new master for Jesus College. Elected to the College Development Committee (July 2000) to advise on college development and fund raising. Director of Studies for Physics and Mathematics for Natural Scientists in Jesus College (1997-2001). My responsibilities include looking after the educational welfare of physics undergraduates at Jesus as well as coordinating the teaching of Physics and Mathematics for natural scientists.

### **Computational Expertise**

I have published research that used large scale computing to address challenge problems in computational chemistry and physics. I am now focused on transferring the techniques and algorithms developed to understand problems in computational/systems biology. As part of our Biomedical Grid initiative in Singapore I have been directing the year long training of grid engineers (53 trained with government funding), building a operational test-bed for biomedical applications and developing new code to run over the grid cyber-infrastructure that links geographically distributed computing and data resources. Ongoing work include porting and tuning key bioinformatics applications such as BLAST, CLUSTALW, CELLWARE onto the Grid.

### **Publications**

#### **Reviews**

W. M. C. Foulkes, L. Mitas, R.J. Needs and G. Rajagopal, "*Quantum Monte Carlo Simulations of Solids*", *Reviews of Modern Physics*. 73 , 33-81, (2001).

M. Nekovee, W.M.C. Foulkes, A.J. Williamson, G Rajagopal, and R.J. Needs, "*A quantum Monte Carlo approach to the adiabatic connection method*", 33, 189, *Advances in Quantum Chemistry*, Thematic volume on DFT, edited by J.M. Seminario, (1999).

W. M. C. Foulkes, R.J. Needs and G. Rajagopal, "*Quantum Monte Carlo Simulations of Real Solids*", *High Performance Computing*. R.J. Allen et. el. (eds), (Kluwer Academic Publishers, Dordrecht, 1999).

R.J. Needs, G. Rajagopal, A.J. Williamson, L.M. Fraser, S.D. Kenny, W.M.C. Foulkes, A.J. James, and P. Maccallum ``*Quantum Monte Carlo studies of electronic systems* ", *J. Korean Physical Society* 29, S116-S120 (1996).

U. Landman, R. Barnett, G. Rajagopal and A. Nitzan, ``*Energetics and Dynamics of Solvation and Fission in Clusters*'', Proceedings of the European Physical Society, Topical Conference on Nuclear and Atomic Clusters, Finland, (1992).

R. Barnett, U. Landman, G. Rajagopal and C. Cleveland, ``*Evolutionary Patterns of Structure and Stability of Clusters*'', NATO Advanced Research Workshop on Physics and Chemistry of Finite Systems : From Clusters to Crystals, Vol. 374, 165, edited by P. Jena, S. Khanna and B. Rao (Kluwer Academic Publishers, Dordrecht, 1992).

R. Barnett, U. Landman, G. Rajagopal and A. Nitzan, ``*Dynamics, Spectra and Relaxation phenomena of excess electrons in Clusters*'', Israel Journal of Chemistry, 30, (1990).

### Articles

S.P. Chia and G. Rajagopal, ``*An exact calculation for the flavor-changing quark-photon vertex*'', Physics Letters, 156B, 405 (1985).

G. Rajagopal, R. Barnett, A. Nitzan, U. Landman, E. Honea, P. Labistie, M.L. Homer and R.L. Whetten, ``*Optical Spectra of Localized excess electrons in Alkali Halide Clusters*'', Physical Review Letters, 64, 2933 (1990).

R. Barnett, U. Landman, A. Nitzan and G. Rajagopal, ``*Born-Oppenheimer dynamics using Density-Functional Theory : Equilibrium and Fragmentation of small Sodium Clusters*'', Journal of Chemical Physics, 94, 608 (1991).

G. Rajagopal, R. Barnett and U. Landman, ``*Metalization of Ionic Clusters*'', Physical Review Letters, 67, 727, (1991).

R. Barnett, U. Landman, and G. Rajagopal, ``*Patterns and Barriers for fission of charged small metal Clusters*'', Physical Review Letters, 67, 3058, (1991).

G. Rajagopal and R.J. Needs, ``*An optimized Ewald method for long-ranged potentials*'', Journal of Computational Physics, 115, 399 (1994).

G. Rajagopal, R.J. Needs, S. Kenny, W.M.C. Foulkes and A. James, ``*Quantum Monte Carlo calculations for solids using special k-points methods*'', Physical Review Letters, 73 1959 (1994).

G. Rajagopal, R.J. Needs, W.M.C. Foulkes, W.M.C. Foulkes, S. Kenny and A. James, ``*Variational and diffusion Quantum Monte Carlo calculations at Non-zero Wavevectors : Theory and application to Diamond-Structure Germanium*'', Physical Review B 51 , 10591 (1995).

S. Kenny, G. Rajagopal and R.J. Needs, ``*Relativistic corrections to atomic energies using quantum Monte Carlo calculations*'', Physical Review A 51 , 1898 (1995).

L. Fraser, W.M.C. Foulkes, G. Rajagopal, and R.J. Needs, ``*Finite-size effects and Coulomb interactions in quantum Monte Carlo calculations for homogeneous systems with periodic boundary conditions*'', Physical Review B 53 , 1814 (1996).

A.J. Williamson, G.Rajagopal, R.J. Needs, L. Fraser, A. James, W.M.C. Foulkes and P. Maccallum, ``*Optimized Wavefunctions for quantum Monte Carlo studies of Atoms and Solids*'', Physical Review B 53 , 9640 (1996).

S.D. Kenny, G.Rajagopal, R.J. Needs, A.J. Williamson, W-K Leung, L.M. Fraser, W.M.C. Foulkes and M.J. Godfrey, ``*Quantum Monte Carlo Calculations of Relativistic Corrections to the Energy of the Homogeneous Electron Gas.*'', Physical Review Letters, 77 1099 (1996).

A.J. Williamson, G.Rajagopal, R.J. Needs, L.M. Fraser, W.M.C. Foulkes Y. Wang and M.-Y. Chou, ``*Elimination of Coulomb finite size effects in quantum many-body simulations.*'', Physical Review B55 R4867 (1997).

R.J. Needs and G. Rajagopal ``*First-principles calculations of the adsorbate-induced surface stress of K/Al(111) ( $\sqrt{3}\times\sqrt{3}$ )R30*'' . Surface Science 372, 179-184 (1997).

R.Q. Hood, M.-Y. Chou, A.J. Williamson, G.Rajagopal, R.J. Needs, W.M.C. Foulkes ``*Quantum Monte Carlo Investigation of Exchange and Correlation in Silicon.*'', Phy. Rev. Letts. 78, 3350, 1997.

W.M.C Foulkes, M. Nekovee, R.Q. Hood, M.Y. Chou, R.J. Needs, G. Rajagopal, A.J. Williamson, "*Quantum Monte Carlo studies of exchange and correlation in solids*", ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 213, 125, 1997.

R.Q. Hood, M.-Y. Chou, A.J. Williamson, G. Rajagopal, and R.J. Needs, "*Exchange and correlation in silicon*", Physical Review B57 8972 (1998).

A.J. Williamson, R.Q. Hood, R.J. Needs, G. Rajagopal ``*Diffusion Quantum Monte Carlo Calculation of the excited states of Silicon*'', Physical Review B57 12140 (1998).

P.R.C. Kent, R.Q. Hood, M.D. Towler, R.J. Needs and G. Rajagopal, "*Quantum Monte Carlo calculations of the one-body density matrix and excitation energies of silicon*", Physical Review B57 15293 (1998).

P. R. C. Kent, Randolph Q. Hood, A. J. Williamson, R. J. Needs, G. Rajagopal, and W. M. C. Foulkes, "*Finite size errors in quantum many-body simulations of extended systems*", Physical Review B59, 1917 (1998).

P.R.C. Kent, R.J. Needs and G. Rajagopal. "*Monte Carlo energy and variance minimization techniques for optimizing many-body wave functions*", Physical Review B59, 12344, (1999).

W.K. Leung, R.J. Needs, G. Rajagopal, S. Itoh and S. Ihara "*Calculations of Silicon Self-Interstitial Defects*", Physical Review Letters 83 , 2351, (1999).

K. C. Huang, R. J. Needs, and G. Rajagopal, Comment on ``*Quantum Monte Carlo study of the dipole moment of CO*'' [J. Chem. Phys. 110, 11700 (1999)], J. Chem. Phys. 112, 4419, (2000).

P.R.C. Kent, M.D. Towler, R.J. Needs and G. Rajagopal, "*Carbon clusters near the crossover for fullerene stability*", Physical Review B62, 15 394 (2000).

Y. Lee, P. Kent, M. Towler, R. Needs and G. Rajagopal, "*Pseudopotentials for Correlated Electron Calculations*", Physical Review B62, 13347, (2000).

R. Gaudoin, M. Nekovee, W. M. C. Foulkes, R. J. Needs and G. Rajagopal, " Inhomogeneous random-phase approximation and many-electron trial wave functions ", Physical Review B63, 115115, (2001).

W.K. Leung, R.J. Needs, G. Rajagopal, S. Itoh and S. Ihara "*Quantum Monte Carlo study of Silicon Self-Interstitials Defects*", VLSI Design, 13(1-4): 229, (2001).

R. Gaudoin, W. M. C. Foulkes, and G. Rajagopal, " Ab Initio Calculations of the Cohesive Energy and Bulk Modulus of Aluminium", J. Phys.: Condens. Matter 14, 8787-8793 (2002).

R.J. Needs, P.R.C. Kent, A.R. Porter, M.D. Towler and G. Rajagopal, "*Quantum Monte Carlo Calculations for Ground and Excited States*", Int. J. Quant. Chem. 86, 218, (2002).

C.M. Tan, V. Bhargava, KH Chiam and G. Rajagopal, "*Hybrid simulations of stochastic reaction-diffusion processes for modeling intracellular signaling pathways*", submitted to IEE Systems Biology, 2005.

KH Chiam and G. Rajagopal, "*Regulation of noise in MAPK cascades*", in preparation for submission to Biophysical Journal, 2005.

## **Honors & Awards**

- Special Merit Pay Allowance, University of Cambridge, (1991-1996, 1999-2004).
- Elected Fellow of Jesus College (1997).
- Awarded National Science Foundation (USA) scholarship to attend Supercomputing Summer School at the Pittsburgh Supercomputing Centre, June 1990.
- Appointed Junior Associate of the ICTP (Trieste, Italy), (1986-1989).
- Director's Research Assistantship, School of Physics, Georgia Tech, (1987-1991).

## **Grants Awarded**

- Awarded S\$800K BMRC grant with Dr. Phillipa Melamad (DBS/NUS) 2005-2008.

- Awarded S\$1.5M (2001-2004) to plan and build a test bed for the Singapore Biomedical Grid (BMG).
- Awarded S\$2.4M (2002-2003) to build up expertise in Grid Computing by the InfoCom Development Authority of Singapore.
- Awarded £250K in June 1996, for 5 years from Hitachi Japan Ltd. to collaborate with Hitachi's Central Research Lab in Tokyo in the project "Atomic Level Simulations of Submicron Devices".
- Three successful awards (1996/1997/1998) from the Joint Research Equipment Initiative (JREI) for enhancing supercomputing hardware and technical support in the Cambridge High Performance Computing Facility. Total of £5.5M of funding awarded.
- Awarded a ROPA grant (£79,729) by the United Kingdom Engineering and Physical Sciences Research Council (jointly with Dr. R J Needs and Dr. M C Payne). (1996-1999). Awarded grant of 215,000 BF under the NATO Collaborative Research Grants Program (Grant number CRG 951105), for joint collaboration with Dr. R. Needs (Cavendish) and Prof. M-Y Chou (Georgia Tech) on "Electron correlations in Solids : The Quantum Monte Carlo Approach". (1996-1998)

### **Affiliations**

Member of IEEE Society (USA).

Member of IEEE Computer Society (USA).

Member of the American Association for the Advancement of Science (USA)

Member of the Biophysical Society