Curriculum vitae

1 Personal details

Name                  CASSAM-CHENAÏ Patrick
Nationality           french
Permanent position    Research director at the French National Center for Scientific Research
Current Responsibilities Director of the “Interface of Mathematics and Complex Systems” research team
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1.1 Tertiary education and distinctions

— Honorary Research Fellow at the University of Western Australia.
— Habilitation to supervise research, University of Nice-Sophia Antipolis, 2003.
— Bronze Medal of the French National Center for Scientific Research 1996.
— Ph. D., Quantum Physics, University of Paris 6, 1992.
— Former student of the École Normale Supérieure rue d’Ulm, (entrance rank : 2, 1986).

1.2 International collaborations

— University of Napolý. Semi-empirical calculations of reaction paths involving polycyclic aromatic
  hydrocarbons. (V. Barone, Italy, 1989).
— IBM Research Center in San Jose. Application of the exterior algebra formalism in quantum chemistry.
  (A.D. McLean, California, USA, 1990).
— University of Western Australia. Collaboration on many problems : Theoretical problems related to the
  ab initio calculation of spin density ; Contribution to the analysis of polarized neutron diffraction
  experiments ; Optimisation of Gaussian functions for molecular fragments ; Development of the
  electronic mean field configuration interaction method, with various fundings including INSU
  competitive grant funding for Franco-Australian collaborations. (G.S. Chandler, M.D. Gould, B.N.
— Université libre of Brussels. Collaboration on the analysis and the prediction of the spectral signatures
  of interstellar or atmospherical molecules, with various fundings including a TOURNESOL competitive
  grant funding for Franco-Belge collaborations. (J. Lièvin, Belgium, since 1993).
— Jet Propulsion Laboratory, NASA. Collaboration on the analysis of methane far-IR spectrum
  measurements, with competitive grant funding from the French Planetology National Programme. (L.
  R. Brown, USA, since 2004).
— Memorial University of Newfoundland. collaboration on the exploitation of the CONVIV code. (P.G. Mezey, Canada, 2005-2008).
— University of South Carolina. Collaboration on geminal methods in quantum chemistry. (V. Rassolov, USA, 2009-2010).

1.3 Assessment of research

Member of the editorial board of: Journal of Mathematical Chemistry.

1.4 Organization of international scientific events


2 Main scientific achievements and interests

2.1 Derivation of the equations defining the CASSCF variational spaces in the n-electron space and related applications


2.2 Rigorous mathematical results on spin-unrestricted wave function.


2.3 A simple answer to the debated question: Can the dipole moment of an ion be calculated at an other point than the centre of mass?


2.4 Contribution to the analysis of polarised neutron diffraction.


2.5 Opening new challenges to overcome flaws in the tentative justification from first principle of Bader’s atoms in molecules.


2.6 On the observable status of potential energy surfaces.


2.7 Applications of computational invariant theory to quantum chemistry.


2.8 Introducing Hopf algebra techniques in quantum chemistry and interpretation of quantum mechanics.


2.9 Development of the GMFCI method and ab initio calculation of high-accuracy rotation-vibration spectra.


2.10 Astrochemistry and astrobiology applications

2.11 Computer codes
1. CONVIV : project administrator and developer (implementation of the VMFCI method).
2. TONTO : developer (implementation of the EMFCI method).
3. BDF : developer (implementation of the EN-MFCI method).