# Curriculum vitae

## 1 Personal details


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| *Name* | CASSAM-CHENAÏ Patrick |
| *Nationality :* | french |
| *Permanent position :* | Research director at the French National Center for Scientific Research |
| *Current Responsabilities :* | 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 Napoly. 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 polarised 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. Figgis, D. Jayatilaka, Western Australia, 1991-2012).
- Université libre of Brussels. Collaboration on the analyzis 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. Liévin, Belgium, since 1993).
- Jet Propulsion Laboratory, NASA. Collaboration on the analyzis 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 Pisa. Collaboration on the calculation of electronic excited states. (G. Granucci, Italy, 2006-2007).
— University of South Carolina. Collaboration on geminal methods in quantum chemistry. (V. Rassolov, USA, 2009-2010).
— University of Beijing. Collaboration on the "Development and application of the MFCI method",several competitive grants. (W. Liu, China, since 2012).

### 1.3 Assesment of research

Member of the editorial board of : *Journal of Mathematical Chemistry*.
Referee for : *Journal of Physics A and B*, *Physics Letter A*, *The Journal of Chemical Physics*, *Journal of Molecular Structure*, *Theoretical Chemical Accounts*, *Coordination Chemistry Reviews*, *Advances in Quantum Chemistry*, *Journal of Condensed Matter*, *Chemical Physics Letters*, *Journal of Mathematical Chemistry*, *Journal of Condensed Matter*, *Journal of Quantitative Spectroscopy and Radiative Transfer*, *EuroPhysics Letters*.

### 1.4 Organization of international scientific events

**"Mathematical Methods for Ab Initio Quantum Chemistry"**
(ninth issues since 2005, University de Nice Sophia Antipolis).

**" Current possibilities and future challenges:**
**for an Equal quantum mechanical treatment of electrons and atomic nuclei in molecular systems "** (2018, Budapest, Hungaria).

## 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

— P. Cassam-Chenaï, *A generalization of the Plücker relations*, Linear and Multilinear Algebra , **31**, p.77-79, (1992).
— P. Cassam-Chenaï, *Variational spaces of electronic calculations in quantum chemistry*, Journal of Mathematical Chemistry, **15**, p.303-321, (1994).
— P. Cassam-Chenaï, Y. Ellinger, G. Berthier, *Induced mapping in the n-electron space and a transformation of valence-bond structures to molecular orbital functions*, Physical Review A , **48**, p.2746-2751, (1993).
— G. Granucci, P. Cassam-Chenaï et Y. Ellinger, *A chemical application of the algebraic concept of internal space*, Journal of Chemical Physics, **108**, p.2538-2544, (1998).

### 2.2 Rigorous mathematical results on spin-unrestricted wave function.

— P. Cassam-Chenaï et G.S. Chandler, *Sur les fonctions de Hartree-Fock sans contrainte*, Comptes-rendus de l'académie des sciences série II, **314**, p.755-757, (1992).

— P. Cassam-Chenaï et G.S. Chandler, *Spin-unrestricted calculations in quantum chemistry*, International Journal of Quantum Chemistry, **46**, p.593-607, (1993).
— P. Cassam-Chenaï, *Symmetrising Broken Symmetry Wave Functions in Quantum Chemistry*, International Journal of Quantum Chemistry, **68**, p.91-101, (1998).
— P. Cassam-Chenaï, *Spin contamination and noncollinearity in general complex Hartree-Fock wave functions*, Theoretical Chemical Accounts, **134** :125, (2015).

## 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 ?

— P. Cassam-Chenaï, F. Pauzat, et Y. Ellinger, *Electronic and vibronic dipole moments of* $CH_2D^+$, Journal of Molecular Structure (Theochem), **330**, p.167-175, (1995).

## 2.4 Contribution to the analysis of polarised neutron diffraction.

— P. Cassam-Chenaï, *Ensemble densities for atoms and molecules I- General theory*, International Journal of Quantum Chemistry, **54**, p.201-210, (1995).
— P. Cassam-Chenaï, S.K. Wolff et G.S. Chandler, *Ensemble densities for atoms and molecules II- Application to* $CoCl_4^{2-}$, International Journal of Quantum Chemistry, **60**, p.667-680, (1996).
— P. Cassam-Chenaï, *Analytical Formulas for the Magnetic Field Produced by a Spin or a Paramagnetic Current density in the case of Gaussian Basis Functions*, International Journal of Quantum Chemistry, **81**, p.11-15, (2001).
— P. Cassam-Chenaï, *Ensemble Representable Densities for Atoms and Molecules III- Analysis of Polarised Neutron Diffraction Experiments when several Zeeman Levels are Populated*, Journal of Chemical Physics, **116**, p.8677-8690, (2002).
— P. Cassam-Chenaï, D. Jayatilaka, *Contributions of the electronic spin and orbital current to the* $CoCl_4^{2-}$ *magnetic field probed in polarised neutron diffraction experiments*, The Journal of Chemical Physics, **137**, p.064107 , (2012).

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

— P. Cassam-Chenaï, D. Jayatilaka, *Some Fundamental Problems with Zero Flux Partitioning of Electron Densities*, Theoretical Chemical Accounts, **105**, p.213-218, (2001).
— P. Cassam-Chenaï, *Frequently asked questions on « Some fundamental problems with zero flux partitioning of electron densities »*, Journal of Mathematical Chemistry, **31**, p.145-153, (2002).
— P. Cassam-Chenaï, D. Jayatilaka, *A complement to « Some fundamental problems with zero flux partitioning of electron densities »*, Theoretical Chemical Accounts, **107**, p.383-384, (2002).

## 2.6 On the observable status of potential energy surfaces.

— P. Cassam-Chenaï, *A Mathematical Definition of Molecular Structure - Open Problem*, Journal of Mathematical Chemistry , **23**, p.61-63, (1998).
— P. Cassam-Chenaï, *On non-adiabatic potential energy surfaces*, Chemical Physics Letters, **420**, p.354-357, (2006).

## 2.7 Applications of computational invariant theory to quantum chemistry.

— P. Cassam-Chenaï, F. Patras, *Symmetry-Adapted Polynomial Basis for Global Potential Energy Surfaces - Applications to XY4 Molecules*, Journal of Mathematical Chemistry, **44**, p.938-966, (2008).
— P. Cassam-Chenaï, G. Dhont, F. Patras, *A Fast Algorithm for the Construction of Integrity Bases Associated to Symmetry-Adapted Polynomial Representations. Application to Tetrahedral XY4 Molecules*, Journal of Mathematical Chemistry, **53**, p.58-85, (2015).

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

— P. Cassam-Chenaï, F. Patras, *The Hopf Algebra of Identical, Fermionic particle systems - Fundamental Concepts and Properties*, Journal of Mathematical Physics, **44**, p.4884-4906, (2003).
— P. Cassam-Chenaï, F. Patras, *Higher order Schmidt decompositions for indistinguishable, overlapping particles*, Physics Letter A, **326**, p.297-306, (2004).
— P. Cassam-Chenaï, *The electronic mean-field configuration interaction method : I. Theory and integral formulas*, The Journal of Chemical Physics, *124*, p.194109-194123, (2006).
— P. Cassam-Chenaï, G. Granucci, *The electronic mean-field configuration interaction method : II. Improving Guess Geminals*, Chemical Physics Letters, **450**, p.151-155, (2007).
— P. Cassam-Chenaï, *Geometric Measure of Indistinguishability for Groups of Identical Particles*, Physical Review A, **77**, p.032103-032109, (2008).
— P. Cassam-Chenaï, V. Rassolov, *The Electronic Mean-Field Configuration Interaction method : III- the p-orthogonality constraint*, Chemical Physics Letters, **487**, p.147-152, (2010).
— T. Perez, P. Cassam-Chenaï, *Generalization of the concepts of seniority number and ionicity* , Journal of Mathematical Chemistry, **56**, p.1428-1436, (2018).
— P. Cassam-Chenaï, *An improved lower bound for the maximal length of a multivector* , Journal of Mathematical Chemistry, **DOI**, 10.1007/s10910-018-0947-9, (2018).

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

— P. Cassam-Chenaï et J. Liévin, *Alternative Perturbation Theory for the Molecular Vibration-Rotation Problem*, International Journal of Quantum Chemistry, **93**, p.245-264, (2003).
— P. Cassam-Chenaï, *Ab Initio Predictions for the Q-Branch of the Methane Vibrational Ground State*, Journal of Quantitative Spectroscopy and Radiative Transfer, **82**, p.251-277, (2003).
— P. Cassam-Chenaï, J. Liévin, *The VMFCI method : A flexible tool for solving the molecular vibration problem*, Journal of Computational Chemistry, **27**, p.627-640, (2006) and supplementary material.
— D. Bégué, C. Pouchan, N. Gohaud, P. Cassam-Chenaï, J. Liévin, *A Comparison of Two Methods for Selecting Vibrational Configuration Interaction Spaces on a Heptatomic System : Ethylene Oxyde*, The Journal of Chemical Physics, **127**, p.164115-164124, (2007) and supplementary material.
— P. Cassam-Chenaï, Yohann Scribano, Jacques Liévin, *Influence of kinetic coupling in rectilinear coordinates on the vibrational spectrum of fluoroform*, Chemical Physics Letters, **466**, p.16-20, (2008).
— P. Cassam-Chenaï, *Rayleigh-Schroedinger perturbation theory generalized to eigen-operators in non-commutative rings*, Journal of Mathematical Chemistry, *49*, p.821-835, (2011).
— P. Cassam-Chenaï, Y. Bouret, M. Rey, S. A. Tashkun, A. V. Nikitin, VL. G. Tyuterev, *Ab initio effective rotational Hamiltonians : A comparative study*, International Journal of Quantum Chemistry,

visible avant impression **112**, p.2201-2220, (2012).

— P. Cassam-Chenaï, A. Ilmane, *Frequently Asked Questions on the mean field configuration interaction method. I- Distinguishable degrees of freedom*, Journal of Mathematical Chemistry, **50**, p.652-667, (2012).

— P. Cassam-Chenaï, J. Liévin, *Ab initio calculation of the rotational spectrum of methane vibrational ground state*, The Journal of Chemical Physics, **136**, p.174309, (2012).

— P. Cassam-Chenaï, J. Liévin, *An improved third order dipole moment surface for methane*, Journal of Molecular Spectroscopy, **291**, p.77-84, (2013) and supplementary material.

— P. Cassam-Chenaï, G. Rousseau, A. Ilmane, Y. Bouret, M. Rey, *Application of quasi-degenerate perturbation theory to the calculation of rotational energy levels of methane vibrational polyads*, The Journal of Chemical Physics, **143**, p.034107 (15 pages), (2015).

— P. Cassam-Chenaï, B. Suo, W. Liu, *Decoupling electrons and nuclei without the Born-Oppenheimer approximation : The Electron-Nuclei Mean-Field Configuration Interaction Method*, Physical Review A, **92**, p.012502 (15 pages), (2015).

— P. Cassam-Chenaï, B. Suo, W. Liu, *A Quantum Chemical Definition of Electron-Nucleus Correlation*, Theoretical Chemical Accounts, **136**, p.52 (12 pages) (2017).

## 2.10 Astrochemistry and astrobiology applications

— P. Cassam-Chenaï , F. Pauzat et Y. Ellinger,*Is stripping of polycyclic aromatic hydrocarbons a route to molecular hydrogen ?*, AIP Conference Proceedings **312** (I. Nenner ed., AIP Press, New York, 1994), p.543-547.

— P. Cassam-Chenaï, *Ab Initio infra red spectra of iron-polycyclic aromatic hydrocarbons compounds : a model case*, Planetary and Space Science, **50**, p.871-876, (2002).

— C. Meinert, S. V. Hoffmann, P. Cassam-Chenaï, A. C. Evans, C. Giri, L. Nahon, U. J. Meierhenrich, *Photonenergy-controlled Symmetry Breaking with Circularly Polarized Light*, Angewandte Chemie, **126**, p.214-218 (2014) and supplementary material.

— C. Meinert, P. Cassam-Chenaï, N. C. Jones, L. Nahon, S. V. Hoffmann, U. J. Meierhenrich, *Anisotropy-guided enantiomeric enrichment in alanine using far-UV circularly polarized light*, Origins of life and Evolution of Biospheres, **45**, p.149-161, (2015) and supplementary material.

— G. Mulas, C. Falvo, P. Cassam-Chenaï, C. Joblin, *Anharmonic vibrational spectroscopy of PAHs*, The Journal of Chemical Physics, **149**, p.144102, (2018) and supplementary material.

## 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).