

Curriculum vitae

Personal details

Name CASSAM-CHENAÏ Patrick
Date of birth 16-12-1965
Nationality : french
Position : permanent research fellow (1st class) at the CNRS,
(Centre National pour la Recherche Scientifique).
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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 de la rue d'Ulm , (entrance rank : 2, 1986).

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, 1990).
- University of Western Australia. On-going 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, 1991-now).
- Université libre of Brussels. On-going 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, 1993-now).
- Jet Propulsion Laboratory, NASA. On-going collaboration on the analyzis of methane far-IR spectrum measurements, with competitive grant funding from the French Planetology National Programme. (L. R. Brown, USA, 2004-now).

MAIN SCIENTIFIC ACHIEVEMENTS

Derivation of the equations defining the CASSCF variational spaces in the n-electron space.

- 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, *Quelques exemples d'application des outils de l'algèbre extérieure à la chimie quantique*, Folia Chimica Theoretica Latina, **XXIII**, p.9, (1995).

Rigorous mathematical demonstration of the fundamental theorem : A spin-unrestricted CASSCF wave function is a spin-restricted CASSCF function if and only if it is an eigenfunction of S^2 . An important corollary is that the ROHF/RHF functions are the only UHF-type (i.e. single determinantal) functions that are eigenfunctions of S^2 .

- 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).

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).

Contribution to the analysis of polarised neutron diffraction experiments. Our general method is the only one to date to have achieved a $\chi^2 < 1$ for the two datas sets collected for the $CoCl_4^{2-}$ with an applied magnetic field parallel and perpendicular to the symmetry axis respectively.

- 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, *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), and document EPAPS N° : E-JCPSA6-116-303218.

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

- 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).

Development of a new, general, variational method for solving the molecular vibrational equation.

Development of a new, general, perturbation method for the obtention of *ab initio*, effective, rotational Hamiltonian.

Prediction of the rotational spectra of methane with unequalled accuracy including intensities.

Energies in cm^{-1} of methane rotational levels in its vibrational ground state

	Carter/Bowman ^a	Wang/Carrington ^b	Wang/Sibert ^c	Cassam-Chenaï/Liévin ^d	STDS ^e
$J = 1$	10.47	10.430	10.44237	10.48165	10.481648
$J = 2$	N/A	N/A	31.32439	31.44213	31.442121
	N/A	N/A	31.32463	31.44240	31.442387
$J = 3$	N/A	N/A	62.64064	62.87581	62.875779
	N/A	N/A	62.64162	62.87689	62.876841
	N/A	N/A	62.64285	62.87824	62.878169
$J = 4 - 18$	N/A	N/A	N/A	largest relative difference 2.10^{-5}	

^a S. Carter et J. M. Bowman, J. Phys. Chem. **A104**, 2355 (2000). MULTIMODE using Lee, Martin and Taylor PES.

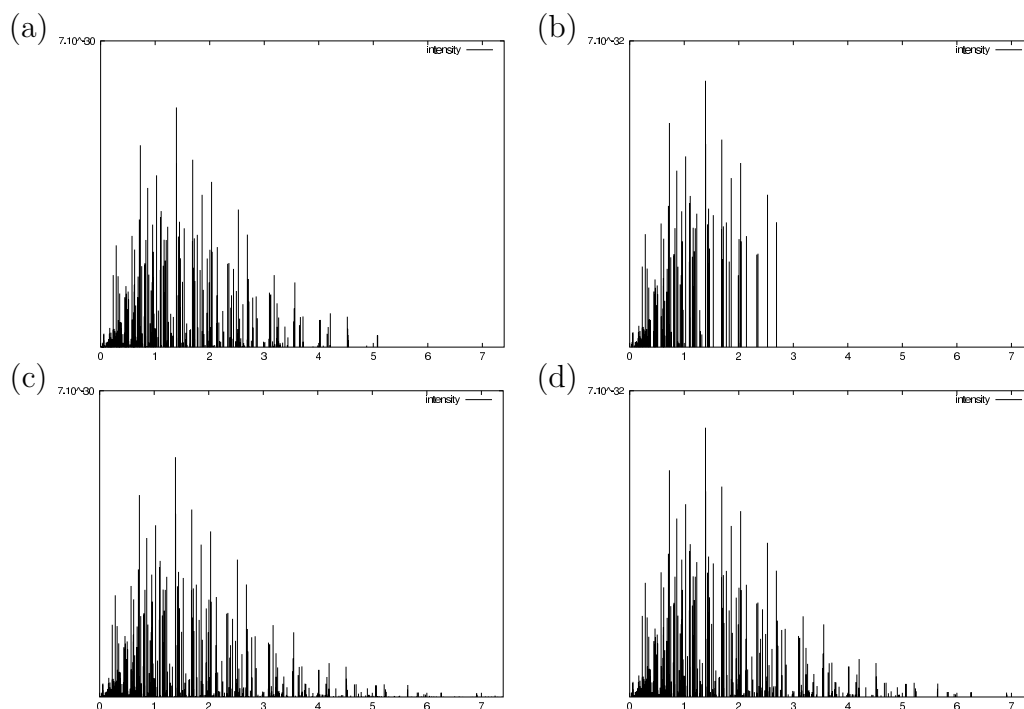
^b X. G. Wang et T. Carrington, J. Chem. Phys **121**, 2937 (2004). CI calculation using Schwenke PES.

^c X. G. Wang et E. L. Sibert, Spectrochimica Acta A **58**, 863 (2002). 12 force constants adjusted on experiment.

^d VMFCI using Lee, Martin and Taylor PES + generalised perturbation with a single parameter related to the equilibrium distance scaled by a factor 1.0002535.

^e C. Wenger and J. P. Champion, J. Quant. Spectrosc. Radiat. Transfer **59**, 471-480 (1998). From an effective Hamiltonian accurate to 10^{-5} cm^{-1} .

Q-Branch of the vibrational ground state of methane at 500K



Comparison of the extrapolation from HITRAN for $^{12}\text{CH}_4$ (a) and $^{13}\text{CH}_4$ (b) with *ab initio* calculated spectra for $^{12}\text{CH}_4$ (c) and $^{13}\text{CH}_4$ (d). Units as in HITRAN, intensities in [$\text{cm}^{-1} / (\text{molecule} \cdot \text{cm}^{-2})$], wave numbers in cm^{-1} .

- 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).
- J. Liévin and P. Cassam-Chenaï, *The vibrational mean-field configuration interaction (VMFCI) method : a flexible tool for solving the molecular vibration problem*, in “International Conference on Computational Methods in Sciences and Engineering 2004”, Lectures Series on Computer and Computational Sciences, Vol. 1, (T. Simos et G. Maroulis Eds. , VSP, Utrecht, Boston, 2004), pp 834-837.

**Introducing Hopf algebra techniques in quantum chemistry.
Application to the generalization of an important theorem for the
interpretation of quantum mechanics. More to be published.**

- 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).

Other contributions

- 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).
- 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.
- P. Cassam-Chenaï, *The real generators of the unitary group*, in. “Strategies and Applications in Quantum Chemistry”, (M. Defranceschi et Y Ellinger eds., Kluwer, 1996), p.77-78.
- P. Cassam-Chenaï, *A Mathematical Definition of Molecular Structure - Open Problem*, Journal of Mathematical Chemistry , **23**, p.61-63, (1998).
- P. Cassam-Chenaï, *Symmetrising Broken Symmetry Wave Functions in Quantum Chemistry*, International Journal of Quantum Chemistry, **68**, p.91-101, (1998).
- 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).
- P. Cassam-Chenaï, D. Jayatilaka, G.S. Chandler, *Gaussian Functions Optimised for Molecules*, Journal de Chimie Physique, **95**, p.2241-2266, (1998).
- P. Cassam-Chenaï, *The exterior algebra : A formalism for fermions in quantum chemistry*, in Recent research developments in quantum chemistry, **2**, (Transworld Research Network, Trivandrum, 2001), p.23-39.
- 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, *Ab Initio infra red spectra of iron-polycyclic aromatic hydrocarbons compounds : a model case*, Planetary and Space Science, **50**, p.871-876, (2002).