Curriculum vitae

1 Personal details

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 - Deputy director of the Quantazur Institute
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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).
- Foreign languages : English ($\frac{23}{24}$ at ACCESS [1]), Chinese (B2 of CECRL [2]).

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, 1993-2015).
- 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, 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).

1. Australian Assessment of Communicative English Skills
2. Cadre Européen Commun de Référence en Langue

— 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, 2012-2017).
— Leader du Task Group 3 du Cost MOLIM: MOLecules In Motion.
— Université Laval. Collaboration on the "Development of seniority non zero, geminal models". (P. Johnson, Canada, 2024-).

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.*
— Jury member of 6 Ph.D, including 3 as reviewer .
— Jury member of 1 HDR
— External expert for the China University Subject Rankings (CUSR) (5^{th} edition organised by the ministry of education of China)
— Contribution to the INSMI prospective report 2014
— Expert Grands Equipements Nationaux en Calculs Intensifs CT8 (2011-2013)

1.4 Supervision of research

— Graduate level students : 2
— Honnours level students : 19
— Master level students : 6
— Ph. D. level students : 2 + 6 (co-supervised)
— Postdoctorate level researchers : 4

1.5 Teaching

— Nankai university, Tianjin (CHINA) : *"From Brown Dwarfs to Hopf algebra : a journey in theoretical chemistry"*, ($3 \times 1.5h$, master level, september 2004).
— Muséum national d'histoire naturelle (Paris) : *"Chimies interstellaires. De l'observation à la modélisation : le rôle de la simulation numérique"* (Master "Evolution, Patrimoine Naturel et Société", december 2004).
— Third Sardinian Summer School of Astrophysics (Italia), *Hands on : Introduction to the MFCI method and the CONVIV code*, (13 h, 30 september- 6 october 2012).
— Northwest University (Xi'an, CHINA) : *"Exterior Algebra Techniques to Compact Information in Fermionic Quantum Systems"*, ($3 \times 2h$, master level, August 2016).
— METEOR (Modules Experiment-ThEOry-Research) entitled "In Silico Astrochemistry" du MAUCA (Master track in Astrophysics in Université Côte d'Azur) (35h, september-october 2024).

1.6 Organization of international scientific events

— **"Mathematical Methods for Ab Initio Quantum Chemistry"** (ninth issues since 2005, University de Nice Sophia Antipolis).
— "Optical Coherence and Quantum Phenomena in Small and Single-Photon Sources: from Fundamentals to Applications - CohQuantSSPhS" (5-7 October 2016, UNS)
— "First European Asymmetry Symposium" (15-16 Mars 2018, Université Côte d'Azur)

— "Current possibilities and future challenges : for an Equal quantum mechanical treatment of electrons and atomic nuclei in molecular system" (2018, Budapest, Hungaria).
— "1st UCA QuantAzur days" (16-17 June 2022, Université Côte d'Azur)
— " UCA-Majulab Workshop 2023 - quantum technologies & photonics" (19-21 June 2023, Université Côte d'Azur)
— "Quantum Probabilities" (14 November 2023, Université Côte d'Azur)
— "2nd UCA QuantAzur days" (14-15 October 2024, Nice)
— "Quantum Control" (14-15 October 2024, Nice)

1.7 Computer codes

— **CONVIV** : project administrator and developer (implementation of the VMFCI method).
— **TONTO** : developer (implementation of the EMFCI method).
— **BDF** : developer (implementation of the EN-MFCI method).

2 Selected contributions over the past five years

2.1 Publications in peer reviewed journals

1. J. Su, B. Suo, P. Cassam-Chenaï, *Theoretical Study of the Anisotropy Spectra of the Valine Zwitterion and Glyceraldehyde*, J. Phys. Chem. **A124**, 6824 (2020).
2. E. Mátyus, P. Cassam-Chenaï *Orientational decoherence within molecules and emergence of the molecular shape*, J. Chem. Phys **154**, 024114 (2021).
3. P. Cassam-Chenaï, G. Lebeau, *Smeared Coulomb potential orbitals : I- Asymptotic expansion* , J. Math. Chem. **59**, 985-1013 (2021).
4. G. Dhont, P. Cassam-Chenaï, F. Patras, *Molien generating functions and integrity bases for the action of the $SO(3)$ and $O(3)$ groups on a set of vectors*, J. Math. Chem. **59**, 2294-2326 (2021).
5. P. Cassam-Chenaï, E. Mátyus, *Electrons as an environment for nuclei within molecules : a quantitative assessment of their contribution to a classical-like molecular structure*, Theor. Chim. Acta. **140**, 159 (2021).
6. P. Cassam-Chenaï, T. Perez, D. Accomasso, *2D-block geminals : A non 1-orthogonal and non 0-seniority model with reduced computational complexity*, J. Chem. Phys **158**, 074106 (2023).
7. P. Cassam-Chenaï, *A conjecture on antisymmetrized geminal power wavefunctions*, J. Math. Chem. **62**, 222-227 (2023).
8. P. Cassam-Chenaï, *Simple conditions for the transformation of dynamical coordinates into canonical ones in Hamiltonian dynamics*, Open Communications in Nonlinear Mathematical Physics **4**, 2 (2024). doi : 10.46298/*ocnmp*.12890
9. P. A. Johnson, J.-D. Moisset, M. Gratton, É. Baril, M.-A. Plourde, M. Lefebvre, M. Kerleaux, P. W. Ayers, P. Cassam-Chenaï, S. De Baerdemacker, D. Van Neck, *Singlet geminal wavefunctions*, Theor. Chim. Acta. **144**, 6 (2025).

2.2 Invited conference talks

1. *"La boite à outils de l'algèbre extérieure pour le problème à N-corps fermionique"*, P. Cassam-Chenaï, (Première réunion générale du GDR NBODY, Lille, France, 8-10 janvier 2020).
2. *"Electrons as an environment for nuclei within molecules : a quantitative assessment of their contribution to a classical-like molecular structure"*, P. Cassam-Chenaï, (Réunion annuelle du GDR ThéMS, webconf, France, 15-16 déc. 2020).

3. *"Invariants and covariants in Quantum Chemistry : applications and open problems "*, P. Cassam-Chenaï, (Workshop : Algebraic Combinatorics of the Symmetric Groups and Coxeter Groups, Cetraro, Italie, 5-9 Juillet 2021).
4. *"2D-block Geminals : Taming the combinatorics while releasing the strong orthogonality constraint"*, P. Cassam-Chenaï, (Workshop : Algebraic Combinatorics and Finite Groups III, Cetraro, Italie, 8-12 Juillet 2024).
5. *"From astrochemistry to geminal theory : a journey under control"*, P. Cassam-Chenaï, (Workshop : New trends in quantum control , Nice, 16-17 October 2024).

2.3 Communications

1. *"NISQ computing : a chemist point of view"*, P. Cassam-Chenaï, (Workshop : "Mathematics for Quantum Technologies", Nice, 4 March 2022).
2. *"Reducing computational cost of geminal methods for strongly-correlated electrons"*, P. Cassam-Chenaï, (JTMS 2022, Rennes, 13-14 Octobre 2022).
3. *"Deciphering the aromatic infrared bands : the LAIBrary project"*, C. Joblin, G. Mulas, K. Demyk, S. Chakraborty, D. Toublanc, E. Ounesli, C. Bastelica, M. Rapacioli, A. Simon, P. Cassam-Chenaï, O. Berné, (Workshop : "Physique et Chimie du Milieu Interstellaire 2022", Paris, 24-28 Octobre 2022).
4. *"Theoretical study of the vibrational spectra of Naphtalene and its cation with the VMFCI method"*, C. Bastelica, P. Cassam-Chenaï, (NanoSpace Joint Scientific Meeting, Ljubljana, 9-11/02/2023, Slovénie).
5. *"2D-block geminals : A non 1-orthogonal and non 0-seniority model with reduced computational complexity"*, P. Cassam-Chenaï, (QUITEL 2023, Montevideo (Uruguay), 26-30 Novembre 2023).

2.4 Seminars

1. *"2D-block Geminals : building on wave functions related to Lewis electron pairs"*, (University of New Brunswick, Fredericton, Canada, 10/05/2024).
2. *"2D-block Geminals : Taming the combinatorics while releasing the "seniority zero" constraint"*, (University of Toronto, Canada, 14/05/2024).
3. *"Taming the combinatorics of antisymmetrized product of geminals"*, (INRIA,Sophia Antipolis, 25/06/2024).