Chérif F. Matta

B.Pharm.Sci., Dipl., PhD, HDR, FRSA, FRSB, FInstP, FRSC, FAAS, FAAAS

* **Professor and Department Chair/Head**,
  Dept. of Chemistry and Physics, *Mount Saint Vincent University*.
* **Adjunct Professor** at *Dalhousie University*, *Saint Mary's University*, and *Université Laval*.
* **Director of Accreditation** & **Member of the Board of Directors,** *Canadian Society for Chemistry* (CSC), *Chemical Institute of Canada* (CIC).
* **Member**, *Commission for Quantum Crystallography – International Union of Crystallography* (IUCr).
* **Member**, *Canadian National Committee for Crystallography* (CNCC).

LANGUAGES

Arabic, English, French, Spanish[a]

EDUCATION AND TRAINING

- **Habilitation to Direct Research (HDR)**,[b] *Université de Lorraine* (France) - (2007-2009)
  Advisor: Prof. Claude Lecomte.
- **Izaak Walton Killam Postdoctoral Fellow**, *Dalhousie University* (Canada) - (2004-2006)
  Supervisor: Prof. Russell J. Boyd.
- **Postdoctoral Fellow**, *University of Toronto* (Canada) - (2002-2004)
  Supervisor: Prof. John C. Polanyi (Nobel Laureate).
- **Doctor of Philosophy (PhD)**, McMaster University (Canada) - (2002)
  Supervisor: Prof. Richard F. W. Bader.
- **Graduate Diploma in Health Services & Hospital Administration**, *National Institute for Higher Management* (Egypt) - (1994).
- **Bachelor of Pharmaceutical Sciences (Hon.)**, *Alexandria University* (Egypt) - (1987).

[a] Publishes and lectures in the four languages.

[b] The HDR is the highest academic degree in France; based on a dissertation and a public defense, it is equivalent to the D.Sc. in the Commonwealth System.

EMPLOYMENT

Dates	Rank/Position	Department	Institution
2021 – 2024 2018 – 2021 2015 – 2018 2009 – 2015 2006 – 2009	Full Professor & Dept. Chair Full Professor Full Professor & Dept. Chair Associate Professor Assistant Professor	Dept. of Chemistry and Physics	*Mount Saint Vincent University*, Halifax, NS, Canada
2006 – 2026	Hon. Adjunct Professor	Dept. of Chemistry	*Dalhousie University*, Halifax, NS, Canada
2011 – present	Adjunct Professor	Dept. of Chemistry	*Saint Mary's University*, Halifax, NS, Canada
2017 – 2025	Adjunct Professor	Dept. of Chemistry	*Université Laval*, Québec City, QC, Canada
2018 – present	Adjunct Professor	Biomedical Sciences Program	*Zewail City of Science and Technology,* Egypt
2016 – 2017	Lady Davis Visiting Professor	The Institute for Drug Research, Faculty of Medicine	*The Hebrew University of Jerusalem*, Israel
2013 (1/3-31/5)	Visiting Scientist	Dept. of Physics and Astronomy	*University College London* (UCL), UK
2011 (1/7–31/8) 2009 (1–31/5) 2007 (1/5–31/8)	Invited Professor Invited Professor Invited Assistant Professor	Laboratoire de Cristallographie, Résonance Magnétique et Modélisations	*Université de Lorraine*, France
2007 (1/5 – 31/8)	Consultant	Laboratory of Quantum Crystallography, Dept. of Chemistry	*Hunter College - City University of New York* (CUNY), New York, NY, USA
2004 – 2005	Adjunct Professor	Dept. of Chemistry	*McMaster University*, Hamilton, ON, Canada
2004 – 2006	Killam Postdoctoral Fellow	Dept. of Chemistry	*Dalhousie University*, Halifax, NS, Canada
2002 – 2004	Postdoctoral Fellow	Dept. of Chemistry	*University of Toronto*, Toronto, ON, Canada
2003 – 2004	Demonstrator	Dept. of Chemistry	*University of Toronto*, Toronto, ON, Canada

Dates	Rank/Position	Department	Institution
1996 – 2001	Teaching Assistant	Dept. of Chemistry	*McMaster University*, Hamilton, ON, Canada
2000	Instructor/Teacher (Finite Mathematics)	OAC (Grade 12) Mathematics	*Southern Ontario College*, Hamilton, ON, Canada
1991 – 1995	Medical Supplies Specialist	Regional Office for the Eastern Mediterranean (EMRO)	*World Health Organization* (*WHO*)
1988 – 1990 (Military service)	First Lieutenant-Pharmacist, Egyptian Navy	Medical Supplies Unit, Division of Medical Services	*Egyptian Navy Headquarters*

AWARDS, PRIZES, HONORS, DISTINCTIONS

Year	Award, Prize, Honor, or Distinction	Body/Institution/Organization
2022-2003	Awarded a *Distinguished Visiting Professorship* under the "*Excellence Initiative - Research University Program (ID-UB)*" by the Polish Minister of Science and Higher Education tenable at Adam Mickiewicz University in Poznań (Poland)	Minister of Science and Higher Education (Poland)
2022-2023	Member Multidisciplinary Selection Board,[a] Canada Excellence Research Chairs (CERC).	The Tri-Council of Canada (Canadian Institutes of Health Research (CIHR), the Natural Sciences and Engineering Research Council of Canada (NSERC), and the Social Sciences and Humanities Research Council of Canada (SSHRC)) - The Government of Canada
2022-2023	Member Comité multidisciplinaire « Microbiologie/Virologie » (Multidisciplinary Committee "Microbiology/Virology"), Fonds de recherche du Québec – Nature et technologies (FRQNT).	Fonds de recherche du Québec – Nature et technologies (FRQNT) - The Government of Quebec
2023-2026	Member Canadian National Committee for Crystallography (CNCC)	CNCC with the National Research Council of Canada (NRC) is the adhering member to the International Union of Crystallography (IUCr)

[a] Described as: "*A diverse multidisciplinary selection board composed of world-leading national and international researchers*" (Link).

Year	Award, Prize, Honor, or Distinction	Body/Institution/Organization
2022	Invited as expert witness before the House of Commons of Canada's Standing Committee on Science and Research - 44th Parliament, 1st Session (Monday, 17 Oct. 2022, 6:30-9:30 p.m.) - to testify on "*Research and Scientific Publication in French*" (Link01; Link02)	The House of Commons, The Parliament of Canada
2021 (announced in 2022 due to COVID)	Elected - Fellow of the African Academy of Sciences (FAAS): "*The AAS Fellowship comprises individuals who have reached the highest level of excellence in their field of expertise and have made contributions to the advancement of the field on the African continent. Fellows of The AAS are elected based on their achievements that include their publication record, innovations, leadership roles and contribution to society*."	African Academy of Sciences (HQ: Nairobi, Kenya)
2021	Elected - Fellow of the American Association for the Advancement of Science (FAAAS): "*For distinguished novel contributions from theoretical and computational chemistry and chemical physics ...*"	American Association for the Advancement of Science, USA
2021 – 2022 2019 – 2021 2018 – 2019	*Chair of the Committee* *Member* *Invitee Member* Canada Research Chairs (CRC) Program's Interdisciplinary Adjudication Committee (IAC) of Canadian Tri-Agency[a]	The Tri-Council of Canada (Canadian Institutes of Health Research (CIHR), the Natural Sciences and Engineering Research Council of Canada (NSERC), and the Social Sciences and Humanities Research Council of Canada (SSHRC)) - The Government of Canada
2021-2022	Science Atlantic "*annual speaker tour of notable scientists*" Speaker of the Year.	Co-sponsored by Science Atlantic and the Chemical Institute of Canada (CIC)

[a] CRC Interdisciplinary Adjudication Committee membership official "Recruitment Principles" read (Link): "*Given the very important role that IAC plays in ensuring accountability and upholding the high level of excellence and prestige of the program, the standards for committee membership are high. Committee members must have:*

- *stature or recognition within the research community as an excellent researcher;*
- *prior experience as a peer review committee member;*
- *excellent judgment; and*
- *the ability to recognize excellence.*"

Year	Award, Prize, Honor, or Distinction	Body/Institution/Organization
2021-2024 2018-2021	*Director of Accreditation* & *Member of Board of Directors* *Member* of the Accreditation Committee Canadian Society for Chemistry	Chemical Institute of Canada (CIC)
2021 – 2022	*Member*, Adjudication Panel B (Sciences and Engineering) African Research Initiative for Scientific Excellence (ARISE) Pilot Programme	The African Academy of Science (Headquarters based in Nairobi (Kenya)).
2019	Elected - Fellow of the Royal Society of Biology (FRSB): "*… made a prominent contribution to the advancement of the biological sciences, and has gained no less than five years of experience in a position of senior responsibility."*	Royal Society of Biology, UK
2018	Ambassador Award (for bringing the Sagamore 2018 Conference to Halifax): "*The Halifax Ambassador Program is a program that honours and works with individuals, who through their association and influence promote, Halifax as a premier meetings and conventions destination.*"	Discover Halifax, City of Halifax, Halifax, Nova Scotia, Canada
2018	Elected - Fellow of Royal Society of Arts (FRSA): *"… an award granted to individuals that the Royal Society of Arts (RSA) judges to have made outstanding achievements to social progress and development. …, the award recognizes the contributions of exceptional individuals from across the world who have made significant contributions relating to the Arts, Manufacture and Commerce."*	Royal Society of Arts (UK)
2018-2021	"Member", Selection Committee (1604) - Research Tools and Instruments (RTI) Grants Program competition for the Chemistry	Natural Sciences and Engineering Research Council of Canada (NSERC)
2017 – 2024	Elected - Member of the "*Commission on Quantum Crystallography*" of the International Union of Crystallography (elected for two consecutive terms + a year COVID-19 extension)	International Union of Crystallography (IUCr)
2017	Award for Research Excellence: "… given to a faculty member on an annual basis. The award recognizes that individual's contribution to the research community and to the research climate at Mount Saint Vincent University. The award also serves to showcase the high level of scholarly research at Mount Saint Vincent University."	Mount Saint Vincent University (Canada)

Year	Award, Prize, Honor, or Distinction	Body/Institution/Organization
2017	Resolution No. 1267 of the Nova Scotia Legislature (pages 2773-2774) [titled: "Matta, Chérif F. - Lady Davis Fellowship", dated: 28 April 2017], in a motion by the Honourable Member Ms. Patricia Arab concludes with the statement: " ... *Whereas Dr. Matta is an outstanding leader in our community and an incredible member of the faculty of Mount Saint Vincent University; therefore be it resolved that the members of this House of Assembly join me on congratulating Dr. Matta on his most recent accolade and wish him well in his future endeavours*".	Nova Scotia Legislature (the legislative branch of the Government of the Province of Nova Scotia).
2016	Elected - Fellow of the Institute of Physics (FInstP): *"…indicates a very high level of achievement in physics and an outstanding contribution to the profession."*	The Institute of Physics (IOP), UK
2016	Lady Davis Visiting Professor & Fellow (Medicine, $7,000) : "The Lady Davis Fellows are selected on the basis of demonstrated talent and promising ideas for their research."	Lady Davis Fellowship Trust, Israel
2016	Laureate of « La preuve par l'image » - Science Exposed Prize (national competition, $2,000) : "Contest Goals" include: "Showcase images of Canadian research."	Natural Sciences and Engineering Council of Canada (NSERC) & Association francophone pour le savoir (Acfas), Québec
2015-2018	Member, Chemistry Evaluation Group (1504) - Discovery (Operating) Grants	Natural Sciences and Engineering Research Council of Canada (NSERC)
2010	Elected - Fellow of the Royal Society of Chemistry (FRSC): "*… must have made an outstanding contribution to the advancement of the chemical sciences; or to the advancement of the chemical sciences as a profession; or have been distinguished in the management of a chemical sciences organization.*"	Royal Society of Chemistry, UK
2009	MGMS Silver Jubilee Prize for 2009: "*...awarded to outstanding young researchers in the field*."	Molecular Graphics and Molecular Simulation Society (MGMS), UK
2004	John Charles Polanyi Prize in Chemistry:	Council of Ontario Universities (COU), The Government of Ontario,

Year	Award, Prize, Honor, or Distinction	Body/Institution/Organization
	Awarded to "*exceptional young researchers*" and consisting of a certificate and personal cash prize of $20,000.	Canada
2004–2006	Izaak Walton Killam Fellow (Chemistry): *"Evaluation Criteria: Excellence in scholarly work and independent research - 60%; Quality of proposed research project - 30%; Personal qualities of the applicant - 10%."*	The Killam Trusts, Canada
2005, 2003	BioVision-Next Science Fellow "Bio-Leaders of Tomorrow": "*Fellowship awarded to 100 of the brightest and most promising PhDs and MBAs from all Universities worldwide*"	American Association for the Advancement of Science (AAAS) & The World Life Science Forum
2003–2004	Chemistry Teaching Fellowship: "*For significant contributions to curriculum development in CHEM447H (4th year biological chemistry)*"	University of Toronto, Canada
2004, 2001	IUCr Young Scientist Travel Awards (obtained twice)	International Union of Crystallography (IUCr)
2003	My paper: Matta, C. F. & Bader, R. F. W. *Proteins: Struct. Funct. Genet.* **52**, 360-399 (2003): Is ranked "***Exceptional (top 1% of selected publication)***" by the Director of the European Bioinformatics Institute, Professor-Dame Janet Thornton for the Faculty of 1000. https://f1000.com/prime/recommendations/all?query=Matta+and+Bader	Faculty of 1000 (F1000), UK
2003	Dept. of Chemistry Nominee for the University Distinguished Thesis Award	McMaster University, Canada
2001	Finalist: Schrödinger Prize	American Chemical Society & the Chemical Computing Group, Inc.
2001	Finalist: "Dean of Science Award for Academic Excellence in Graduate Work"	School of Graduate Studies, McMaster University
2001	Centennial Scholarships for Academic Excellence	McMaster University, Canada

BIBLIOMETRIC DATA

RESEARCH SCORES	
Google Scholar (Link)	**Research Gate (Link1, Link 2)**
• *Citations* = **8,847** • *H-index*[a] = **46**. • *i10-index*[b] = **97**.	• *Citations* = **7,859** • *H-index*[a] = **43** • *Research Items* = **192** • *Reads* = **29,693** • *Recommendations:* **709** • *Research Interest Score* = **4,013 -** *This Score* is "***higher than 98% of researchers***".
Included in the list of top world scientists from all disciplines	
• **Ranked 43,797 (top 0.6% worldwide) out of 7 million from all disciplines from 1998-to-2018.** • See SI in: Ioannidis JPA *et al.* (2019) "A standardized citation metrics author database annotated for scientific field" *PLoS Biol* **17**(8): e3000384. https://data.mendeley.com/datasets/btchxktzyw/1 (**Table-S4-career-2018.xtsx**).	
TEACHING SCORES	
Rate My Professor (Link)	
• **Overall Quality = 4.6/5.0** (**average of 82 student ratings).** • **Top Tags for this Professor: (how students describe this professor):** *Inspirational; Respected; Amazing lectures; Hilarious; Caring.*	

SCHOLARLY SERVICE

Membership in National & International Committees

- "*Official Nominator (by invitation only)*" (2023) for the **Kyoto Prize** - (The Japanese equivalent of the "Nobel Prize" – ¥100,000,000 Japanese Yen (approx. $1M).

- "*Nominator (by invitation)*" (2023) for the **Gregori Aminoff Prize** (awarded by the Royal Swedish Academy of Sciences).

- "*Chair/Head of the Committee*" (2021-2024) "*Member*" (2018-2021) of the **Canadian Society for Chemistry (CSC) Accreditation Committee** - (The committee that evaluates and grants the CSC accreditation for chemistry programmes in Canada and around the world). [Workload/experience: Approx. 10 departments of chemistry evaluated / year].

- "*Member*" (2022-2023), Multidisciplinary Selection Board, **Canada Excellence Research Chairs (CERC)** of the Canadian Tri-Council (The Government of Canada) - (The national committee that adjudicates the applications for *Canada Excellence Research Chairs*).

[a] Number of publications with at least that many citations.
[b] Number of publications cited at least 10 times in the last 5 years.

[Workload/experience: Approx. 20 Nominations evaluated / year]

- "*Chair/Head of the Committee*" (2021-2022), "*Member*" (2019-2021), "*Invitee Member*" (2018-2019), of the **Canada Research Chairs (CRC)** Program's Interdisciplinary Adjudication Committee (IAC) of Canadian Tri-Council (The Government of Canada) - (The national committee that adjudicates the applications for *Canada Research Chairs*). (Link)
  [Workload/experience: Approx. 35 Nominations evaluated / year]

- Member, Adjudication Panel B (Sciences and Engineering), African Research Initiative for Scientific Excellence (ARISE) Pilot Programme, **The African Academy of Science (AAS)** (2021-2022).
  [Workload/experience: Approx. 10 grants evaluated per year, in addition to in-person interviewing 50% of the 80-90 finalist candidates].

- Judge/Adjudicator for the Pan-African Prize: *Olusegun Obasanjo Prize for Scientific Discovery and/or Technological Innovation,* **The African Academy of Science (AAS)** (2022).

- Referee/Adjudicator for two nominations for **Fellow of the Royal Society of Chemistry** (FRSC, UK) - (2022, 2021).

- Member, comité multidisciplinaire « Microbiologie/Virologie » (Multidisciplinary Committee "Microbiology/Virology"), **Fonds de recherche du Québec – Nature et technologies (FRQNT)** (2022-2023) - (Committee that evaluates research grants on behalf of the government of the Province of Quebec).
  [Workload/experience: Approx. 5-6 grants evaluated / year].

- Member of the Selection Committee (1604) for Research Tools and Instruments (RTI) Grants Program competition (Chemistry) of the **Natural Sciences and Engineering Research Council of Canada (NSERC)** (2018-2021) - (The national grant selection committee that evaluates grants for infrastructure in Chemistry in Canada).
  [Workload/experience: Approx. 30 grants evaluated / year].

- Member of the Chemistry Evaluation Group (1504) of the **Natural Sciences and Engineering Research Council of Canada (NSERC)** (2015-2018) - (The national grant selection committee that evaluates operating grants in Chemistry in Canada). (Link)
  [Workload/experience: Approx. 40-50 grants evaluated / year].

- Member of the Commission on Quantum Crystallography of the **International Union of Crystallography (IUCr)** (2017-2024 two consecutive terms + a year COVID19 extension). (Link)

- Member of the Canadian National Committee for Crystallography (CNCC). The CNC with the National Research Council of Canada (NRC) is the adhering member to the

International Union of Crystallography (IUCr).

- Member of the Expert Review Committee on Chemistry, Biochemistry and Biophysics of the **Compute Canada Federation** (2021-2022) - (The committee that evaluates and grants strategic CPU time allocations on the Compute Canada Grid). Invited to serve another year (2022-2023) but declined due to overcommitment.
  [Workload/experience: Approx. 12 grants evaluated / year].

- Member of the *"Extended Pool of Panel Members"* (2019 – open ended) of the **Research Foundation – Flanders (Belgian Public Research Council)** - (*Fonds Wetenschappelijk Onderzoek – Vlaanderen* (FWO)).

- Evaluator for *"Frontier Science 2019"* - **CONACYT (National Council of Science and Technology (of Mexico))**.

Consulting

- "*Panelist*" – (defined as "expert to help us ensure that the definitions included are the industry standard") for the *Future Medicinal Chemistry Glossary*, Future Medicinal Chemistry in partnership with Future Drug Discovery and the associated website *Rx Net* (2019).

- "*Consultant*" of the Commission on Charge, Spin and Momentum Densities of the International Union of Crystallography (IUCr) (2015-2017).

- "*Consultant*" at the Laboratory of Quantum Crystallography, Dept. of Chemistry, Hunter College, City University of New York, New York, NY, USA. (1 May - 31 August 2007).

Reviewing Service to Research Funding Agencies and Organizations
(Year(s) of service as a Reviewer/Referee are in brackets)

- *Referee for Central and North American Research Funding Agencies:*
  - *Office of Basic Energy Sciences (BES) of the Department of Energy (DOE) - Office of Science (USA)* (2020).
  - *American Chemical Society (ACS) Petroleum Research Fund* [2020, 2018].
  - *Consejo Nacional de Ciencia y Tecnología (CONACYT) [Nacional Council of Science and Technology] of Mexico]* [2020].
  - *Natural Sciences and Engineering Council of Canada (NSERC)* [2018, 2013 (twice, once for chemistry and once for physics), 2012 (twice), 2011, 2009, 2007].
  - *National Science Foundation (NSF - USA)* (2018, 2015, 2012, 2011).
  - *US Department of Energy - Office of Science (DOE - USA)* (2016).
  - *Fundación Marcos Moshinsky (Foundation Marcos Moshinsky), Mexico* (2015).
  - *US Army Research Office (USA)* (2011).

- *Referee for South American Research Funding Agencies:*
  - *Comisión Nacional de Investigación Científica y Tecnológica (CONICYT),* Chile (2017, 2015).

- *Referee for European Research Funding and Universities:*
  - Referee for the "Advanced Laureate Awards Programme (IRCLA)" of the *Irish Research Council (IRC)* [*An Chomhairle um Thaighde in Éirinn*], Republic of Ireland – (2023).
  - Referee for an "Émergence" Proposal, *Sorbonne Universié*, France – (2023).
  - *Engineering and Physical Sciences Research Council,* UK (EPSRC) (2022, 2017, 2009, 2007).
  - *Swiss National Science Foundation (FNSNF) (Switzerland),* SNFS Ambizione program for early career scientists (2022).
  - *Research Commission of the Swiss Federal Institute of Technology (ETH−Zürich)* (2020, 2016, 2015, and 2011).
  - *Swiss National Science Foundation (FNSNF) (Switzerland),* Research Grant (2019).
  - *National Science Center (Poland),* (3 grants to review in 2019).
  - *The Research Foundation - Flanders (FWO), (Belgium): Operating Research Grants* (2018, 2014, and 2012).
  - *The Research Foundation - Flanders (FWO), (Belgium): Postdoctoral Fellowship Awards* (2018, 2017).
  - *French National Research Agency* (ANR) (2017).
  - *National Science Centre - Poland* OPUS (Requested to act as a Reviewer twice in 2016, accepted once).
  - *Foundation for Polish Science (Fundacja na rzecz Nauki Polskiej, FNP)* HOMMING (2016).
  - *Romanian Executive Agency for Higher Education, Research, Development and Innovation Funding (UEFISCDI)* (2016).
  - Referee for *LabEx MiChem – Comité Scientifique, Université Pierre et Marie Curie – Sorbonne Universités* (2015-2016).
  - External evaluator of a candidate for the Appointment to the Rank of Professor for *Universität Bremen (Institut für Angewandte und Physikalische Chemie)* (2015).
  - *Czech Science Foundation "Grantová agentura České republiky – GACR"* (2015, 2014 (twice), 2012).
  - *The Excellence Initiative, Postdoctoral-Initiative of the University of Bremen (Germany)* (2013).
  - *The European Commission: Marie Curie Fellowships (EU, Brussels)* (2013, 2012).
  - *The Levrhulme Trust,* UK (Referee No. 92785), (2021, 2004).
  - *Royal Society of Chemistry* (RSC), UK (ReSourCe ID # 218763), since 2006.

- *Referee for African Research Funding Agencies:*
  - African Academy of Science (AAS) (2021 (5 reviews), 2022 (2 reviews))
  - *National Research Foundation (NRF) of South Africa* (2022, 2016, 2013, 2011 (twice))

- *Referee for Middle-Eastern Funding Agencies:*
  - *KAUST Supercomputing Laboratory (KSL) - King Abdullah University of Science and Technology (KAUST), Kingdom of Saudi Arabia*. Computer time allocation proposal (2019).
  - *Israel Science Foundation (ISF)* (2017)

- *Other Refereeing:*
  - *Evaluator for the Gordon Research Conferences (GRC 2013)* on Electron Distribution & Chemical Bonding (2013).
  - Judge for *Academia Europaea (Academy of Europe) Prizes for Young Russian Scientists* (2013).

Peer-Review / Refereeing Service for Journals
(Average 10±5 review requests/month)

Frequent Reviewer for: *Accounts of Chemical Research*, *ACS Omega*, *Acta Crystallographica B, American Mineralogist, Angewandte Chemie International Edition, Arabian Journal of Chemistry, Australian Journal of Chemistry, Bioorganic & Medicinal Chemistry Letters, Biochimica et Biophysica Acta (BBA) - General Subjects, Canadian Journal of Chemistry, Carbon, Chemical Communications (ChemCom), ChemMedChem, ChemPhysChem, Chemical Physics*, *Chemical Physics Letters*, *Chemical Science, Comptes Rendus Chimie*, *Computational and Theoretical Chemistry, Computational Biophysics and Chemistry, Crystal Growth and Design*, *Dyes and Pigments*, *Foundations of Chemistry, Electronic Structure, European Journal of Inorganic Chemistry, European Journal of Medicinal Chemistry, Heliyon, International Journal for Light and Electron Optics, Industrial & Engineering Chemistry Research, International Journal of Quantum Chemistry*, *Israel Journal of Chemistry, Journal of Biomolecular Structure & Dynamics, Journal of Chemical Education*, *Journal of Chemical Physics, Journal of Chemical Theory and Computation, Journal of Cluster Science, Journal of Computational Chemistry, Journal of Mathematical Chemistry, Journal of Molecular Graphics & Modeling, Journal of Molecular Liquids, Journal of Molecular Modeling, Journal of Molecular Structure, Journal of Molecular Structure: THEOCHEM (Continued since 2011 as: Computational and Theoretical Chemistry), Journal of Organic Chemistry, Journal of Physical Chemistry (A and B)*, *Journal of Physical Organic Chemistry, Journal of Physics and Chemistry of Solids, Journal of the American Chemical Society*, *Journal of the Brazilian Chemical Society*, *Materials Chemistry and Physics*, *Mendeleev Communications*, *Molecular Physics*, *Nanoscale, National Academy Science Letters, Nature Communications*, *New Journal of Chemistry*, *Nuclear Science and Techniques*, *Organic & Biomolecular Chemistry, Physica A, Physical Chemistry Chemical Physics (PCCP)*, *Physica Scripta*, *PLoS One*, *Polish Journal of Environmental Studies*, *Proceedings of the National Academy of Sciences of the United States* (PNAS), *RSC Advances, Symmetry,* and *Theoretical Chemistry Accounts*.

Peer-Review / Refereeing Book Proposals:

2023:

- Sason Shaik, David Danovich, and Philippe C. Hiberty: *A Chemist's Guide to Valence Bond Theory, Second Edition*, John Wiley and Sons– (monograph) (2023).

2021:

- R. Nalewajski: *Chemical Reactivity in Quantum Mechanics and Information Theory*, Elsevier– (monograph) (2022).
- Anderson, J. S. M.; Cortés-Guzmán, F.; Rodríguez, J. I. (Eds.) *Advances in Quantum Chemical Topology Beyond QTAIM*, , Elsevier, The Netherlands – (edited collection) (to be published in 2023).

2017:

- L. Piela: *Ideas of Quantum Chemistry, Third Edition*, Elsevier (2021) – (monograph). [Book published in 2017].

2009:

- N. Sukumar: *A Matter of Density*, Elsevier (2013) – (edited collection).

Reviewing Promotion & Tenure Professorial Applications & Senior Administrative Hires

- Committee Chair, Dept. Chemistry and Physics Re-appointment Committee for Lab Instructors (DRCLI) for the re-appointment of a Laboratory Instructor, Mount Saint Vincent University (Canada) – (2023).
- External Referee for the promotion to the Rank of Associate Professor in Chemistry (in Physical Chemistry), King Abdulaziz University (Kingdom of Saudi Arabia) – (2021).
- Member, Dept. Chemistry and Physics Appointment Committee for Lab Instructors (DRCLI) for the hiring of a Laboratory Instructor, Mount Saint Vincent University (Canada) – (2021).
- External Referee for the promotion to the Rank of Full Professor in Chemistry, Lakehead University (Canada) – (2020).
- Member, Director of Facilities Management Search Committee, Mount Saint Vincent University (Canada) – (2020).
- Member, Tenure Review Committee, Laboratory Instructor, Dept. of Chemistry and Physics, Mount Saint Vincent University (Canada) – (2018).
- Member, Department Review Committee for Promotion to Full Professor, Dept. of Biology, Mount Saint Vincent University (Canada) – (2017-2018).
- Member, Department Review Committee for Hiring Laboratory Instructor, Dept. of Chemistry and Physics, Mount Saint Vincent University (Canada) – (2014).
- Member, Department Review Committee for Promotion to Full Professor, Dept. of Chemistry and Physics, Mount Saint Vincent University (Canada) – (2013-2014 – Twice (two promotions)).
- Member, Department Review Committee for Promotion to Associate Professor with Tenure, Dept. of Chemistry and Physics, Mount Saint Vincent University (Canada) – (2007).
- Member, Jeanne Sauvé Award Selection Committee, Mount Saint Vincent University (Canada) – (2014).

Site Visits for Departmental Adjudications:

- Canadian Accreditation Site Visit Team Representative of the Canadian Society of Chemistry to evaluate the Department of Chemistry, Sultan Qaboos University, Muscat (Sultanate of Oman) – (24-27 Dec. 2022).
- Canadian Accreditation Site Visit Team Representative of the Canadian Society of Chemistry to evaluate the Department of Chemistry, Qatar University, Doha (Qatar) – (8-10 April 2021). (Via zoom due to the COVID19 pandemic).
- Canadian Accreditation Site Visit Team Representative of the Canadian Society of Chemistry to evaluate the Department of Chemistry, Jordan University of Science and Technology (JUST), Irbid (The Kingdom of Jordan) – (23 Feb. – 1 March, 2020).
- Internal Reviewer to evaluate the Department of Cultural Studies, Mount Saint Vincent University (Canada) – (2020).

Editorial Boards

- Associate Editor: *Foundations of Chemistry* (Springer) (2021-present).
- Member of the Editorial Board: *Foundations of Chemistry* (Springer) (2014-2021).
- Member of the Editorial Board: *Molecules* (MDPI-Switzerland) (2021-present).
- Member of the Editorial Board: *BioEssays* (Wiley) (2019-present).
- Member of the Editorial Board: *Future Medicinal Chemistry* (Future Science Group) (2008-present).

ORGANIZING CONFERENCES AND SYMPOSIA

30 Member of the International Scientific Committee, 46th annual *Congress of Theoretical Chemists of the Latin Expression Quitel XLVI* (**CHITEL / QUITEL 2023**), (26-30 November 2023), Montevideo, Uruguay. (Link)

29 Member of the International Scientific Advisory Committee, *8th International Conference: Nanobiophysics: Fundamental and Applied Aspects*, **NBP-2023** (3-6 October 2023), Institute of Physics of the National Academy of Science of Ukraine (NAS), Kiev, Ukraine. (Link)

28 Co-Organizer (with Dr. S. Sowlati-Hashjin) of: *Symposium on Chemical Effects of Electric Fields; 106th Canadian Chemistry Conference and Exhibition* ***CSC 2023***, (4 – 8 June 2023), Vancouver, BC, Canada.

27 Member of the International Advisory Committee, *9th European Charge Density Meeting:* ***ICDM9 2022***, (13-17 June 2022), Aarhus University, Aarhus, Denmark. (Link)

26. Member of the Program Committee, *7th International Conference: Nanobiophysics: Fundamental and Applied Aspects*, **NBP-2021** (4-8 October 2021), Institute of Physics of the National Academy of Science of Ukraine (NAS), Kiev, Ukraine. (Link)

25 Co-organizer (with Dr. Anna Makal) of Microsymposium 220 on "Quantum crystallographic studies on intra/inter-molecular interactions" at the *Congress and General Assembly of the International Union of Crystallography IUCr-2021*, Prague, Czech Republic, 14-22 August 2021. (Link)

24 Co-organizer (with Prof. Paul W. Ayers and Prof. Farnaz H. Zadeh) of the Symposium "*Frontiers in Chemical Understanding and Prediction: New Descriptors and Concepts for Chemical Phenomena*" at the *48th International Union of Pure and Applied Chemistry (IUPAC) World Chemistry Congress and 51st IUPAC General Assembly*, (13-20 August, 2021), Montreal, Canada. (Link)

23. Co-organizer (with Prof. Jacob Overgaard) of a one day Session, Discussion Leader (with Prof. Overgaard) of a forum on "Frontiers in Quantum Crystallography", and Judge for the Conference Poster Prize at the *Quantum Crystallography Online Meeting 2020 QCrOM2020 (International Union of Crystallography – Commission on Quantum Crystallography)*, (August 26 - 29, 2020).

22 Member of the International Scientific Advisory Committee, *6th International Conference: Nanobiophysics: Fundamental and Applied Aspects*, **NBP-2019** (1-4 October 2019), Institute of Physics of the National Academy of Science of Ukraine (NAS), Kiev, Ukraine. (Link)

21. Member of the Scientific Advisory Committee, *International Charge Density Meeting: **ICDM 2019***, (21-26 July 2019), Georg-August-Universität Göttingen, Germany. (Link)

20. Organizer (with Prof. Gilles Peslherbe and Prof. Pierre-Nicholas Roy) of the 45th annual *Congress of Theoretical Chemists of the Latin Expression Quitel XLV* (**CHITEL / QUITEL 2019**), (25-30 August 2019), Montreal, Canada. (Link)

19. Member of the "Honorary Committee", *Quantum International Frontiers 2018 Conference*, (17-21October 2018), Hunan Province, China.

18. Chair and Organizer of the ***Sagamore XIX (2018)** Conference on Quantum Crystallography of the International Union of Crystallography (IUCr)*, (8-13 July 2018), Halifax, Canada.[a]

17. Organizer of: *Symposium on Electron Localization and Delocalization: Theory, Measures, and Applications in Chemistry; 100th Canadian Chemistry Conference and Exhibition **CSC 2017***, (28 May – 1 June 2017), Toronto, ON, Canada.

16. International Advisory Board Member: *ChemBond 2016: Chemical Bonding in Position Space*, Max Planck Institute for Chemical Physics of Solids, Dresden, 2016 (November 27 - December 1, 2016).

15. Member of the Scientific Advisory Board and the International Organizing Committee: *7th European Charge Density Meeting **ECDM7***, of the European

[a] Received the 2018 Ambassador Award from the City of Halifax for bringing Sagamore 2018 Conference to Halifax (with delegates from 27 countries).

Crystallographic Association, Warsaw June 2016.

14. Member of the International Programme Committee: *3rd International Interdisciplinary Symposium, **CroArtScia2015** – Technological Innovations: Art & Science* (27–30 May 2015), Zagreb, Croatia.

13. Co-organizer (with Dr. Birger Dittrich) of Microsymposium on "MS-65 Charge Density for Drug Design" at the *Congress and General Assembly of the International Union of Crystallography **IUCr-2014***, Montreal 5-12 August 2014. (49 submitted abstracts).

12. Member of the International Organizing Committee: *Asymmetry: Art & Science & Education, International Scientific Interdisciplinary Symposium, **CroArtScia 2013*** (8–11 May 2013), Zagreb, Croatia.

11. Organizer of a "*Session in Honor of Professor Richard F. W. Bader"* at the *Sagamore XVII Conference on Electron Charge, Spin and Momentum Densities, International Union of Crystallography **IUCr-2012***, (15–20 July 2012), Hokkaido, Japan.

10. Member of the International Advisory Committee, *6th European Charge Density Meeting **ECDM6***, (15 – 20 September 2012), Štrbské Pleso, Slovakia.

9. Member, Organizing Committee: *Second International Conference on Nanobiophysics: Fundamental and Applied Aspects*, (6-9 October 2011), Kiev, Ukraine.

8. Member of the International Organizing Committee: *International Scientific Symposium Symmetry: Art and Science, **CroArtScia 2011*** (4–7 May 2011), Zagreb, Croatia.

7. Session President (Président de session): "Concepts in Chemistry", *Epistémologie de la chimie : synthèse et perspectives (Epistemology of Chemistry: synthesis (philosophical synthesis) and perspectives)*, École Polytechnique – CREA (Centre de recherche en épistémologie appliquée), CNRS - UMR 7656, Paris – France, 11 Sept. 2010.

6. Discussion Leader on: Electron Distribution and Interaction Energies, *Gordon Research Conference (**GRC**) on Electron Distribution & Chemical Bonding* (11-16 July 2010).

5. Member of the Organizing Committee of the Mount Saint Vincent University's Conference on Peace: *Being the Change: Building a Culture of Peace in our Classrooms, our Communities, and our World*: Halifax, NS, Canada (7-9 July 2010).

4. Co-Organizer (with Prof. Paul Ayers) of: *Symposium on Atoms in Molecules, 92nd Canadian Chemistry Conference and Exhibition **CSC 2009***, (30 May 30 – 3 June 2009), Hamilton, ON, Canada.

3. Co-organizer (with Prof. Richard F. W. Bader) of a *Symposium on Static and Dynamic Aspects of Charge Density*, *5th European Charge Density Meeting **ECDM5***, June 6-11 2008, Gravedona, Italy.

2. Organizer, *Symposium on Bio-Computational Chemistry, 90th Canadian Chemistry*

*Conference and Exhibition **CSC 2007***, May 26 - 30, 2007, Winnipeg, MB, Canada.

1. Member, Organizing Committee of the *Symposium on the Occasion of the 65th Birthday of Prof. Richard Bader*, Burlington, ON, Canada (18-20 Oct. 1996).

PROFESSIONAL MEMBERSHIP

- *African Academy of Sciences* (Fellow (FAAS), elected in 2021 – announced 2022).
- *American Association for the Advancement of Science (USA)* (Fellow (FAAAS), elected in 2021 – announced 2022, Member since 2016).
- *Royal Society of Chemistry (UK)* (Fellow (FRSC), elected in 2010).
- *Institute of Physics (IoP, UK)* (Fellow (FInstP), elected in 2016).
- *Royal Society of Biology (UK)* (Fellow (FRSB), elected in 2019).
- *Royal Society of Arts (UK)* (Fellow (FRSA), admitted in 2018).
- *American Physical Society (APS, USA)* (Member since 2016).
- *Association francophone pour le savoir – Section Acadie (Acfas-Acadie, Québec, Canada)* (Member since 2022).
- *Association francophone pour le savoir (Acfas, Québec, Canada)* (Member since 2016).
- Union des professeurs de physique et de chimie (UDPPC, Paris, France) (Member since 2017).
- *Sigma Xi, The Scientific Research Society (USA)* (Member, elected in 2005)
- *American Chemical Society (ACS, USA)* (Member since 2001)
- *The Chemical Institute of Canada (CIC, Canada)* (Member since 2003)
- *Canadian Society for Chemistry (CSC, Canada)* (Member since 2003).
- *Canadian Society of Biochemistry, Molecular and Cellular Biology (CSBMCB, Canada)* (Regional Representative since 2010-2012).

SUPERVISION OF HIGHLY QUALIFIED PERSONNEL (HQP) & Theses

Visiting Professors

- Dr. Zahir Hussain, PhD - Professor, Dept. of Physiology, Faculty of Medicine, Umm Al-Qura University (UQU), Saudi Arabia (2020).
- Dr. Anna Gubskaya, PhD, Rutgers University (2010-2011).

PhD Theses

- Marianne Kerleaux (to start in January 2024), PhD Thesis, Dept. of Chemistry, Laval University. (Co-supervised with Prof. Paul Johnson).
- Peyman Fahimi (2019-2023), PhD Thesis, Dept. of Chemistry, Laval University. *Theoretical Investigations in Mitochondrial Biophysics.* (Co-supervised with Prof. T. Tung Nguyen-Dang).

- Lázaro Andrés Monteserín Castanedo (2019-2023),[a] PhD Candidate (Saint Mary's University, thesis submitted, awaiting thesis defence): *Some Applications of the Topographical Analysis of the Electron Density in Quantum Biochemistry*.
- Alya A. Arabi, *PhD Thesis* (Dalhousie University, 2008-2012): *Density Functional Theory: Dispersion Interactions & Biological Applications*. (Co-supervised with Professor Axel D. Becke).
- Hugo Bohórquez, *PhD Thesis* (Dalhousie University, 2007-2011): Local Quantum Chemistry. (Co-supervised with Professor Russell J. Boyd).

Visiting PhD Students

- Halis Yenis Seuret Hernández, Visiting PhD Student, PhD Candidate at Universidad Autónoma del Estado de Morelos (UAEM) (Cuernavaca, Mexico) - Emerging Leaders in the Americas Program (ELAP) Scholar (Government of Canada) – (1 Sept. 2023 – 29 Feb. 2024).
- Mal Hedrick (September 2022-August 2023), Visiting PhD Student, Saint Mary's University.
- Cyrus Ahmadi Toussi (January-December 2019), Visiting PhD student, Biomedical Engineering (Bioelectrics), Hakim Sabzevari University, Sabzevar, Iran. (Co-supervised with Prof. J. Haddadnia, Hakim Sabzevari University).
- Luiz Alberto Terrabuio, *PhD Thesis* (São Paulo University, 2016). (Co-supervised by Prof. R. L. Haiduke, Sao Paolo University, Brazil).[b]

MSc Theses

- Islam K. Matar, *MSc Thesis* (Saint Mary's University, started in Sept. 2023, in progress): (Tentative) *Bioinformatics Study of Bacterial Resistance to Antibiotics*.
- Lázaro Andrés Monteserín Castanedo, *MSc Thesis* (Saint Mary's University, started in 2019, in progress): *Some Applications of the Topographical Analysis of the Electron Density in Quantum Biochemistry*.
- Youji Cheng, *MSc Thesis* (Saint Mary's University, 2017-2019): *A Computational Investigation of the Intrinsic Field of ATP Synthase*.[c]
- Ismat Sumar, *MSc Thesis* (Saint Mary's University, 2013-2016): *Localization-Delocalization Matrices: Theory and Applications*. (Co-supervised with Professor Paul W. Ayers).
- Shahin Sowlati Hashjin, *MSc Thesis* (Saint Mary's University, 2011-2013):[d] *Computational Investigations of Some Molecular Properties, their Perturbation by*

[a] Lázaro Castanedo is the Winner of the 2020 Abe Leventhal Student Research Award (Alzheimer Society of Nova Scotia), winner of a Scotia Scholars Award for 2019, winner of a Poster Prize at International Union of Crystallography's (IUCr)'s Conference - Sagamore 2018, winner of an Emerging Leaders in the Americas Program (ELAP) Scholarship (Government of Canada), and winner of a Wood-Whelan Research Fellowships of the International Union of Biochemistry and Molecular Biology (IUMB).

[b] Supported by a "*Brazilian Science without Frontiers*" Programme Scholarship.

[c] Chosen as Valedictorian for the graduating class in the May 2020 convocation.

[d] Nominated for the Governor General Gold Medal by the examining committee.

External Electric Fields, and their use in Quantitative Structure-to-Activity Relationships.

Honors Theses

- Ailish Sullivan, *Honors Thesis* (Dept. of Chemistry & Physics - Mount Saint Vincent University), co-supervised with Prof. Tina Harriott (2023-2024): *Quantum Chemical Spectroscopy of Interstellar Small Molecules as Carriers of Diffuse Interstellar Bands*.
- Emily Smith, *Honors Thesis* (Dept. of Mathematics - Mount Saint Vincent University), co-supervised with Prof. Tina Harriott (2021-2022): *Reddening of Diffuse Interstellar Bands (DIBs) and the Thickness of Interstellar Dust Clouds*.
- Fraser Smith, *Honors Thesis* (Dept. of Mathematics - Mount Saint Vincent University), co-supervised with Prof. Tina Harriott and Prof. Daniel Majaess (2020-2021): *Diffuse Interstellar Bands (DIBs) Correlations as a Means to Identify new Molecular Carriers*.
- Mohamed Ahmed Nasr El-Deen, *Honors Thesis* (Zewail City of Science and Technology, 2018-2019): *DNA-Histone Interaction, a Computational Study*.
- Hebatallah Emam, *Honors Thesis* (Zewail City of Science and Technology, 2018-2019): *Effects of the Electric Field across the Inner Mitochondrial Membrane on some Molecules and Reactions of the Electron Transport Chain (ETC)*.
- Mennatallah Emam, *Honors Thesis* (Zewail City of Science and Technology, 2018-2019): *Molecular Fingerprinting in Quantitative Structure-to-Activity Relationships (QSARs) as Tool in Drug Design*.
- Mathew Timm, *Honors Thesis* (Joint Dalhousie University - Mount Saint Vincent University Honors Programme, 2013-2014): *What Happens to the Chemical Bond if a Bonded Atom Undergoes a Nuclear Transformation? A Computational Study*.[a]
- Alya A. Arabi, *Honors Thesis* (Joint Dalhousie University - Mount Saint Vincent University Honors Programme, 2007-2008): *Atomic Partitioning of the Energy of Reaction: The Hydrolysis of a Fuel Biological Molecule, Adenosine 5'-Triphosphate*.

Research Associates, Research Assistants & Visiting Students

- Yan (Helena) Xing, Mount Saint Vincent University's IBIS (International, Black, and International Students) Programme - Undergraduate Research Assistant (2022-2023) co-supervised with Prof. Tina Harriott (Summer 2022): *Diffuse Interstellar Bands (DIBs)*.
- Ailish Sullivan, *NSERC-USRA Undergraduate Research Assistant*, (Summer 2023): *Diffuse Interstellar Bands (DIBs)*.
- Ailish Sullivan, *Undergraduate Research Assistant*, co-supervised with Prof. Tina Harriott (Summer 2022): *Diffuse Interstellar Bands (DIBs)*.
- Carson Cameron, *Jeanne Sauvé Award Scholar* ($6,500) - *Research Assistant*, (Summer 2022): *Mitochondrial Biophysics*.
- Austin Bray, *Directed Reading Summer Student*, co-supervised with Prof. Tina Harriott

[a] Matthew Timm has been awarded the *Science Atlantic Communication Award* at the *Science Atlantic/CIC Annual Student Chemistry Conference* (ChemCon 2014) for an oral presentation based on this Honors Thesis.

(Summer 2022): *Spectroscopy of Diffuse Interstellar Bands (DIBs)*.
- Emily Smith, *Graduate Research Assistant*, co-supervised with Prof. Tina Harriott (Summer 2022): *Diffuse Interstellar Bands (DIBs) Correlations*.
- Tiffany Fields, *Research Associate* (Summer 2021, summer 2022): *Diffuse Interstellar Bands (DIBs) Project.*
- Fraser Smith, *Graduate Research Assistant*, co-supervised with Prof. Tina Harriott (Summer 2021): *Diffuse Interstellar Bands (DIBs) Correlations*.
- Emily Smith, *Jeanne Sauvé Award Scholar* ($6,500) - *Research Assistant*, co-supervised with Prof. Tina Harriott (Summer 2021): *Diffuse Interstellar Bands (DIBs) Correlations*.
- Lahcene Azzouz (Winter Semester 2019), Visiting Graduate (senior PhD) Student from Université de Laghouat (Algeria). (Field: Physics of materials).
- Lázaro Andrés Monteserín Castanedo (1 July - 31 October 2016), Visiting Graduate Student on a *Wood-Whelan Research Fellowship Award* ($4,900) from the *International Union of Biochemistry and Molecular Biology* (on visit from the Dept. of Biology, University of Havana).
- Lázaro Andrés Monteserín Castanedo (1 Feb. - 1 July 2017), Visiting Graduate Student on a *Emerging Leaders in the Americas Program Award* ($9,700) from the *Canadian Bureau for International Education* (on visit from the Dept. of Biology, University of Havana).
- Andrea Perrault (Summers of 2016 and 2017), Research Assistant (co-supervised with Prof. Tina Harriott.
- Leanne Ingram (Summer, 2014), Research Assistant, Mount Saint Vincent University.
- Mathew Timm (Summer, 2014), Research Assistant, Mount Saint Vincent University.
- Mathew Timm (Summer, 2013), NSERC-USRA undergraduate research summer student, Mount Saint Vincent University.
- Martin Sichinga (2010-2011), Research Assistant, Mount Saint Vincent University.
- Leigh Herman David (summer semester, 2009), Research Assistant, Mount Saint Vincent University.
- Daniel MacKeigan (summer semester, 2009), Research Assistant, Mount Saint Vincent University.
- Alya A. Arabi (2006-2009), Research Assistant, Mount Saint Vincent University.

BSc Equivalent

- Jack MacGillivary (Winter, 2019), Directed Research Student (Theoretical Investigations in Mitochondrial Bioenergetics), Mount Saint Vincent University.
- Mathew Timm (Fall, 2012), Directed Study Student, Mount Saint Vincent University.
- Seth Robert King (Fall, 2011), Directed Study Student, Mount Saint Vincent University.
- Martin Sichinga (2009-2010), Directed Research Student, Mount Saint Vincent University.

MEMBERSHIP IN THESES COMMITTEES & SERVICE AS EXTERNAL EXAMINER

D.Sc. Dissertation

- D.Sc. External Referee/Evaluator - Dr. Ol'ha Brovarets', *Microstructural Mechanisms of the Origin of the Spontaneous Point Mutations*, Institute of Molecular Biology and Genetics, *National Academy of Sciences of Ukraine* (Kyiv, Ukraine) - (Defense: 29 Dec. 2015).

PhD Theses

- PhD Thesis External Examiner – Salima Hennani, *Simulation numérique des processus d'excitation et d'ionisation des systèmes moléculaires à plusieurs électrons en champ laser intense* [Trans.: Numerical simulation of the excitation and ionization processes of multi-electron molecular systems in an intense laser field], Départment de Chimie, Université Laval, Québec, QC (Canada). (Defense: Fall 2023).
- PhD Thesis External Examiner – G. Pandimuthu, *Synthesis, Characterization, Biological Activity and Corrosion Inhibition Performance of Some Schiff Bases*, Department of Chemistry, Kandaswami Kandar's College, Periyar University, Velur, Tamilnadu, India. (Defense: Fall 2022).
- PhD Thesis Referee and External Examiner – Stuart Raymond Colenzo von Berg, *Bonding Interactions in Congested Molecules: A Study of the Interatomic Forces and the Molecular Electrostatic Potential*, Faculty of Science at Stellenbosch University, South Africa. (Defense: May 2022).
- External Examiner: PhD Comprehensive Exam (Examen de Candidatura) – Yoshio Alan Torres Barrera, *Chemical Reactivity Descriptors: One-Parameter, Two-Parameters, and Dual Descriptors*, Instituto de Química, Universidad Nacional Autónoma de México, (Exam held on: 25 June 2021).
- PhD Thesis Assessor and External Examiner – Florian Kleemiss, *Development of Quantum-Crystallographic Methods for Chemical and Biochemical Applications*, Department of Chemistry and Biochemistry, *Bern University*, Berne, Switzerland. (Defense: Dec. 2020).
- PhD External Referee - Prakash Loknaeh Verma, *Exploring Noncovalent Interactions in Ionic Liquids from Theory*, Dept. of Chemistry, *Savitribai Phule Pune University*, Pune, India. (Defense: Oct. 2019).
- PhD External Examiner - François Dion, *Dynamique de systèmes polyatomiques et polyélectroniques en champ laser intense* (Dynamics of Polyatomic and Polyelectronic Systems in Intense Laser Fields), Dép. de chimie, *Université Laval*, Québec, Canada. (Defense: April 2018).
- Member of PhD Committee and Examiner - Walter Polkosnik, *Fast Geometry Optimizations of Large Systems with the Kernel Energy Method (KEM),* Dept. of Chemistry, Hunter College, *The City University of New York (CUNY)*, USA. (Defense: April 2018).
- PhD External Examiner – P. Tamilselvi, *Kinetics and Mechanism of Oxidation of Aniline and its Substituents Catalysed by Iron(III) Phthalocyanine Chloride*, Anna University,

Chennai, India. (Defense: March 2018).

- PhD External Examiner - Pinaki Saha, *Application of Electron Density-Based Analysis in the Study of Nanoclusters and Biomolecular Interactions*, Dept. of Chemistry, School of Natural Sciences, Shiv Nadar University, India. (Defense: Dec. 2017).
- PhD External Examiner - Hadieh Monajemi, *Proton tunnelling in some proton transfer reactions*, Institute of Graduate Studies, University of Malaya, Malaysia. (Defense: Aug. 2017).
- PhD External Examiner - S. K. Periyasamy, *Oxidation of Chalcones and Thioacids by Quinalidinium Fluorochromate*, Dept. of Chemistry, *National College (Autonomous) - Bharathidasan University*, Tiruchirappalli, India. (Defense: August 2012).
- PhD External Examiner - Andrea Millen, *Properties of C-Linked C8-Phenoxyl Guanine DNA Adducts*, Dept. of Chemistry and Biochemistry, *University of Lethbridge*, Canada. (Defense: Aug. 2011).
- PhD External Examiner - James S. M. Anderson, *From Wavefunctions to Chemical Reactions: New Mathematical Tools for Predicting the Reactivity of Atomic Sites from Quantum Mechanics*, Dept. of Chemistry, *McMaster University*, Canada. (Defense: Nov. 2010).
- PhD External Examiner - Jacob Sanford, *Calculation of Static and Dynamic Effects on the Magnetic Tensors of Several Benchmark Radicals*", Dept. of Chemistry, *University of New Brunswick*, Canada. (Defense: March 2010).
- PhD External Examiner - Po Yang, *Indicator Functions and Their Applications in Fractional Factorial Designs*, Dept. of Mathematics and Statistics, *McMaster University*, Canada. (Defense: July 2004).

M.Sc. Theses

- External Examiner – Pooya Afaghi, *Microwave System for Biophysical Studies*, Dept. of Physics, *Mount Allison University*, Canada. (Defense: Dec. 2018).
- External Examiner - Alexander H. Morrison, *Muon Radiation Chemistry Towards Applications in Modern Reactor Design*, Dept. of Chemistry, *Mount Allison University*, Canada. (Defense: July 2018).
- Member of MSc Thesis Committee & Examiner - Dijana Anželj, *An Ab Initio Investigation of Lead (II) Complexes as Possible Corrosion Products in a CANDU Supercritical Water-Cooled Reactor (SCWR)*, Dept. of Chemistry, *Saint Mary's University*, Canada. (Defense: April 2016).

B.Sc. Honors Theses Examiner

(At Dalhousie University, in the capacity of Adjunct Professor at the Dept. of Chemistry)

- Thomas Burns, *A Computational Comparison of Dithiolene and Diselenolene Ligands for Use in Biomimetic Catalysis* (2013).
- Hilary Matthews, *A Computational Study of the Selective Inhibition of Malaria-Causing Proteins in the Human Body* (2013).
- Tavia Raiche-Marsden, *Site Directed Mutagenesis of Escherichia Coli Cytidine 5'-Triphosphate Synthase in Order to Reduce Steric Bulk in the Active Site and increase*

Synthetic Availability (2013).

- Daniel M. Chevrier, *Properties of Iron / Iron Oxide Nanoparticles and their Biomedical Applications* (2011).
- Wai-Ho Lo, *Examining the Effect of Temperature on Self-discharge and Charge Redistribution in Carbon-based Electrical Capacitors* (2011).
- Elias Machaalani, *A Model for Assessing Solvation Effects of Amino Acids* (2010).
- Daniel Veldhuijzen van Zanten, *How to make Analogs of Carnosine, using AM1 and Molecular Mechanics, that better Chelate Ca^{2+} and Zn^{2+} Ions* (2009).

ACADEMIC VISITORS TO THE RESEARCH GROUP

- Dr. Obed Ogega, Senior Programme Officer, African Academy of Sciences, Nairobi, Kenya (May-June 2022).
- Professor Lou Massa, City University of New York, USA (November 2019).
- Dr. Carlo Gatti, Institute of Molecular Science and Technologies ISTM, Italian National Research Council (July 2018).
- Professor Fernando Cortés Guzmán, Instituto de Química, Universidad Nacional Autónoma de México (UNAM) (July 2018).
- Dr. Ronald Cook, TDA Research Inc., Colorado, USA (July 2018).
- Professor Lou Massa, City University of New York, USA (July 2018).
- Professor Paul W. Ayers, McMaster University, Hamilton, ON, Canada (August 2016).
- Professor Jesus Hernandez-Trujillo, UNAM, Mexico (July 2016).
- Professor Fernando Cortes-Guzman, UNAM, Mexico (July 2016).
- Dr. Ronald Cook, TDA Research Inc., Colorado, USA (June 2016).
- Professor Lou Massa, City University of New York, USA (May 2016).
- Professor Paul W. Ayers, McMaster University, Hamilton, ON, Canada (September 2015).
- Dr. James Anderson, Riken, Japan (September 2015).
- Dr. Ronald Cook, TDA Research Inc., Colorado, USA (September 2015).
- Professor Ada Yonath,[a] Weizmann Institute f Science, Israel (May 2014).
- Professor Lou Massa, City University of New York, USA (May 2014).
- Professor Lou Massa, City University of New York, USA (June 2013).
- Professor Claude Lecomte, Université de Lorraine, France (May 2013).
- Professor André Dieter Bandrauk, Université de Sherbrook, Canada (November 2012).
- Professor Jesus Hernandez-Trujillo, UNAM, Mexico (June-July 2012).
- Dr. Renato Bensasson, Emeritus Directeur of Research at the CNRS, National Museum of Natural History, France (October 2011).
- Professor Gérald Monard, Université de Lorraine, France (May-June 2011).
- Professor Claude Lecomte, Université de Lorraine, France (April 2011).
- Professor Ignacy Cukrowski, University of Pretoria, South Africa (May 2010).
- Professor Anna Gubskaya, Rutgers University, USA (September 2009 – September 2010).

[a] Nobel Laureate in Chemistry (2009).

- Dr. Adrian Culf, Atlantic Cancer Research Institute, Canada (February 2010).
- Professor Lou Massa, City University of New York, USA (October 2008).

TEACHING EXPERIENCE

List of Courses Taught and Years/Semesters Taught

(Listed in decreasing course numbers)
[F = Fall, W = Winter, SS-I = Summer Session I]

GRADUATE COURSES TAUGHT AS INSTRUCTOR/PROFESSOR

CHEM 705: **Computational Chemistry** (*McMaster University*)
[2004 F]

CHEM 6690: **Directed Study in Chemistry/Physics** (*Saint Mary's University*)
Topics in Mathematics and Physics: Classical Mechanics [2018 F]
Advanced Quantum Mechanics [2014 W]
Advanced Quantum Mechanics [2012 F]

CHEM 6691: **Directed Study in Chemistry** (*Saint Mary's University*)
The Quantum Theory of Atoms in Molecules [2011 F]

UNDERGRADUATE COURSES TAUGHT AS INSTRUCTOR/PROFESSOR

MATH 4447: **Directed Study in Mathematics** (*Mount Saint Vincent University*)
Relativistic Thermodynamics [2015 F]

CHEM 4601: **Directed Research in Chemistry** (*Mount Saint Vincent University*)
Theoretical Investigations in Mitochondrial Bioenergetics [2019 W]

CHEM 3502/BIOL 3502: **Intermediary Metabolism** (*Mount Saint Vincent University*)
[2019 W, 2018 W, 2017 W, 2015 W, 2014 W, 2011 W, 2010 W, 2009 W, 2008 W, 2007 W]

CHEM 3501/BIOL 3501: **Introductory Biochemistry** (*Mount Saint Vincent University*)
[2018 F, 2015 F, 2014 F, 2012 F, 2011 F, 2010 F, 2009 F, 2008 F, 2007 F]

CHEM 4990/MATH 4990: **Honors Thesis** (*Mount Saint Vincent University*)

2007-2008	Alya A. Arabi (CHEM)
2013-2014	Matthew Timm (CEHM)
2020-2021	Fraser Smith (co-supervised with Prof. Tina Harriott) – (MATH)
2021-2022	Emily Smith (co-supervised with Prof. Tina Harriott) – (MATH)
2023-2024	Ailish Sullivan (co-supervised with Prof. Tina Harriott) – (CHEM)

BMS 364: **Biophysics** (*University of Science and Technology at Zewail City*)
[2021, Spring]

MATH 3500/PHYS 3500: **Topics in Mathematics and Physics** (*Mount Saint Vincent University*)
The Mathematics of Electromagnetic Theory [2023 W]
UV/Vis and Vibrational Spectroscopy and Group Theory [2022 W]
Classical Mechanics and Dynamics [2015 F]

MATH/PHYS 3500: **Directed Study in Mathematics-Physics** (*Mount Saint Vincent University*)
Computational Spectroscopy [2022 W]

CHEM 3011: **Directed Study in Chemistry** (*Mount Saint Vincent University*)
Chemical Applications of Information Theory [2023 W]
Computational Spectroscopy [2022 SS1]

CHEM 3012: **Directed Study in Chemistry** (*Mount Saint Vincent University*)
Quantum Chemistry [2012 F, 2008 W]

PHYS 3310: **Directed Study in Physics** (*Mount Saint Vincent University*)
Special Relativity Theory [2016 SS-I]
Introduction to Information Theory [2015 W]
Quantum Mechanics [2011 F]

CHEM 3301/PHYS2310: **Introductory Quantum Chemistry/Modern Physics**
(*Mount Saint Vincent University*)
[2019 F, 2017 F, 2016 W, 2014 W, 2012 W, 2010 W, 2007 F]

CHEM 2302: **Chemical Kinetics and Dynamics** (*Mount Saint Vincent University*)
[2011 W, 2009 W, 2007 W]

CHEM 2301: **Chemical Thermodynamics** (*Mount Saint Vincent University*)
[2006 F]

PHYS 2210: **Waved and Optics** (*Mount Saint Vincent University*)
[2020 F, 2014 F, 2012 F, 2010 F, 2008 F]

PHYS 2200: **Electricity and Magnetism** (*Mount Saint Vincent University*)
[2023W, 2021 W, 2019 W, 2011 F, 2009 F]

PHYS 1102: **General Physics II: Electricity and Magnetism**
(*Mount Saint Vincent University*)
[2022 W, 2021 W, 2015 W]

COURSES TAUGHT AS DEMONSTRATOR, TEACHING ASSISTANT, TUTOR

CHM 447H: **Biological Chemistry**
(*University of Toronto*)
[2003 F - to - 2004 W]
Capacity: Chemistry Teaching Award Winner (for contribution

to the Design of a Lab for this course).

CHM 138 Lab: **Introductory Organic Chemistry**
(*University of Toronto*)
[2003 F - to - 2004 W]
Capacity: Demonstrator, Lab Instructor.

PHYS 138: **Physics for the life Sciences**
(*University of Toronto / PREP 101*)
[2003 F - to - 2004 W]
Capacity: Instructor/Tutor for a large class of *PREP 101, Inc.*, Toronto, ON, Canada.

22 LABS: **General Chemistry, Kinetics, Thermodynamics, Physical Chemistry**
(*McMaster University*)
[1996 W - to - 2001 F]
Capacity: Lab Teaching Assistant (TA) and Lab Reports Marker

COURSES TAUGHT AS HIGH SCHOOL TEACHER

OAC-Mathematics: **Ontario Advanced Credit (OAC) in Finite Mathematics**
(*Southern Ontario College, Hamilton, ON, Canada*)
[2000 W]
Capacity: Teacher/Instructor.

UNIVERSITY ADMINISTRATIVE SERVICE

Dates	Role	Committee or Department	Institution
2021 – 2024 2015 – 2018	Department Chair[a]	Dept. of Chemistry and Physics	*Mount Saint Vincent University*
2023	Chair	Dept. Chemistry and Physics Re-Appointment Committee for Lab Instructors (DRCLI) for the re-appointment of a Laboratory Instructor	*Mount Saint Vincent University*
2021 – 2024	Member	University Review Committee (URC) (The committee reviewing promotions and tenure applications of Faculty for final recommendation to the President and Vice Chancellor)	*Mount Saint Vincent university*
2021	Member	Dept. Chemistry and Physics Appointment Committee for Lab Instructors (DRCLI) for the hiring of a Laboratory Instructor	*Mount Saint Vincent University*

[a] *Significant achievement:* Led the successful department's application for the accreditation of its undergraduate major and honors programs from the *Canadian Society for Chemistry* (CSC) in 2016.

Dates	Role	Committee or Department	Institution
2020 –2021	Member	Committee on Research and Publication (CRP) (The committee adjudicating internal research grants and research awards)	*Mount Saint Vincent university*
2020	Faculty Association Representative	Hiring Team for "Director of Facilities Management"	*Mount Saint Vincent University*
2020	Internal Reviewer	Cultural Studies Programme	*Mount Saint Vincent University*
2020	External Appraiser	Application for promotion to Full Professor – Dept. of Chemistry	*Lakehead University*
2017-2020	Member	University Senate	*Mount Saint Vincent University*
2017-2020	Member	Senate Executive Committee	*Mount Saint Vincent University*
2017-2020	Member	Senate Tributes Committee (Adjudicates and recommends Honorary Doctorates to the Senate).	*Mount Saint Vincent University*
2019	Member	Tier II Canada Research Chair (CRC) In Neuroscience Search Committee 2019	*Mount Saint Vincent University*
May-June. 2019	Acting Chair	Dept. of Chemistry and Physics	*Mount Saint Vincent University*
2018	Member	Dept. of Chemistry and Physics Tenure Review Committee for the Dept.'s Laboratory Instructor	*Mount Saint Vincent University*
2015- 2018	Member (Ex-Officio)	Laboratory Safety Committee	*Mount Saint Vincent University*
2017-2018	Member	Dept. of Biology Review Committee (DRC) for the promotion to Full Professor	*Mount Saint Vincent University*
2014-2016	Member	Committee on Academic Policy and Planning (CAPP)	*Mount Saint Vincent University*
2013-2014	Member	Dept. of Chemistry and Physics Review Committee (DRC) for the promotion of Faculty Member B to Full Professor	*Mount Saint Vincent University*

Dates	Role	Committee or Department	Institution
2013-2014	Member	Dept. of Chemistry and Physics Review Committee (DRC) for the promotion of Faculty Member A to Full Professor	*Mount Saint Vincent University*
2014	Member	Dept. of Chemistry and Physics Review Committee (DRC) for the hiring of Laboratory Instructor	*Mount Saint Vincent University*
2013-2015, 2007-2011	Library Rep.	Dept. of Chemistry and Physics	*Mount Saint Vincent University*
2014	Member	Jeanne Sauvé Award Selection Committee	*Mount Saint Vincent University*
Aug. 2008, May 2010	Acting Chair	Dept. of Chemistry and Physics	*Mount Saint Vincent University*
2009–2011	Science Rep.	Committee on Research and Publication (CRP)	*Mount Saint Vincent university*
2009–2011	Member	Joint Saint Mary's University - MSVU Animal Care Committee	*Saint Mary's University and Mount Saint Vincent university*
2006–2009	Member	Joint Occupational Health and Safety Committee	*Mount Saint Vincent university*
2006	Member	Faculty Re-Appointment Committee, Dept. of Chemistry	*Mount Saint Vincent university*
2007	Member	Dept. Review Committee (Promotion and Tenure)	*Mount Saint Vincent university*
2000-2001	Graduate Rep.	Board of Governors	*McMaster University*

TV PROGRAMMING FOR PUBLIC DISSEMINATION OF SCIENCE

TV Host in the Mount Saint Vincent distance learning "Conversation with Faculty" (30 minutes interviews):

- A conversation with Professor Lou Massa (City University of New York) entitled "*Quantum Crystallography*". (Aired in the fall of 2008 on TV Channel 33).
- A conversation with Professor Russell J. Boyd (Dalhousie University) entitled "*Computational Chemistry*". (Aired in the fall of 2009).

INTERVIEWS & MEDIA PROFILES

- ***Est-ce qu'on est en train de perdre le français dans les sciences ? [Trans : Are we losing the French language in sciences?]*** Radio interview with Philippe-Vincent Foisy, OMNY-FM Radio (Montreal):, 8:58–9:07 AM - 11 May 2023 (9.33 minutes). (Link).
- **On the NEWS in *CHEMISTRY WORLD*: *"Electric field of ATP synthase suggests enzyme has functions beyond catalysis"- 28 Feb. 2022*:** Reporting on the discovery in the paper: Vigneau, J.-N.; Fahimi, P., Ebert, M.; Cheng, Y.; Tannahill, C.; Muir, P.; Nguyen-Dang, T.-T. Matta, C. F. "*ATP synthase: A moonlighting enzyme with unprecedented functions*", *ChemComm* **58**, 2650-2653 (2022).
- ***Technology and Thought Leadership in Nova Scotia - The Discover Halifax Podcast :*** A 32 min. interview with Chérif F. Matta by presenter Paul Bailey on intellectual leadership in Halifax. (Link1(Apple Podcasts), Link2(Spotify)). (2021).
- ***Discover Halifax - Success Stories:*** **Video-clip feature with Chérif Matta**, Chair of the International Union of Crystallography Conference Organized in Halifax in 2018. (Link). (2021).
- ***Chemistry and Engineering News (C&E News):*** Invited to comment on the paper: S. Shaik *et al.* "*Oriented External Electric Fields: Tweezers and Catalysts for Reactivity in Halogen-Bond Complexes*", *J. Am. Chem. Soc.* **141**(17), 7122-7136 (2019) → "*Theoretical study proposes that the applied field would hold reactants in place and stretch halide bond*", by Sam Lemonick (*C&EN* Vol 97(15), April 10, p. 9 (2019)).
- **NEWS 95.7 Radio** – The Sheldon MacLeod Show - Monday 9 July 2018 (2:45 – 12:55 pm), interview on "Quantum Crystallography" on the occasion of the International Union of Crystallography (IUCr)'s Conference Sagamore 2018 taking place in Halifax that week.
- **CBC Radio** at Prime time (8:15-8:30 am) Friday 6 July 2018 Interview by Portia Clark "Information Morning" on Quantum Crystallography on the occasion of the IUCr Conference Sagamore 2018 in Halifax the following week.
- **In print interview** of Chérif Matta: "Ask the experts – Computational Chemistry", *Future Medicinal Chemistry* (2018), [Q&A with interviewer Benjamin Walden, Managing Editor of *Future Science Group* and co-interviewee Michael C. Hutter of the Center for Bioinformatics in Saarbrücken]. (*Fut. Med. Chem.* **10***,* 1521-1524).
- **Profiled in *Folia Montana***, Issue of Fall 2017, p. 14 (Research Profile: The Mount's 2017 Research Excellence Award Winner – Chérif Matta).
- **TV Interview on Radio-Canada TV** on 8 May 2016 with TV host Charles Tisseyre entitled "Les Liaisons ingénieuses" (in French) on "La preuve par l'image" NSERC-ACFAS prize (Link).

ART AND SCIENCE

- NSERC-Acfas science image of the year by Chérif F. Matta (Link) included in a 3-month (Aug. - Oct., 2021), Public Square Exhibition – Ottawa. (Link)

- NSERC-Acfas award winning science image "*Les Liaisons Ingénieuses*" by Chérif F. Matta (Link) was selected for inclusion in the NSERC-sponsored exhibition of Award-Winning Science Photography at Mount Saint Vincent University (20th-27th) November 2017. (Link)
- 2016 National NSERC-Acfas Award winner for "*Les Liaisons Ingénieuses*" by Chérif F. Matta (Link).
- Participated in the organization of conferences on Arts, Mathematics, and Science in, Croatia, *CroArtScia* 2015, *CroArtScia* 2013, and *CroArtScia* 2011. (Link)
- Artistic science-inspired abstract oil painting. Works included in juried (refereed) exhibitions and sole shows. (Link)

SERVICE TO COMMUNITY

- Member of the Board of Acfas-Acadie (representing Nova Scotia) (Acadian/Maritime section of Acfas, the principal French-language learned society in Canada). (2023)
- Board of Trustees of *Dalhousie Legal Aid Services (DLAS)*, Halifax, Canada. (Organization that provides legal services for low-income residents of Halifax):
  - Chair of the Board (Jan.-Dec. 2011).
  - Vice Chair of the Board (Jan.-Dec. 2010).
  - Member (2007-2009).
- "*Member*", Environmental Workgroup of the *Ontario Public Health Association* (OPHA) (2002 - 2004).

List of Works & Dissemination of Research Results

Summary of Research Outcomes Dissemination Activities:

	Work	Total
1.	**Publications**	**176**
1.1	Books (2 edited and 2 monographic)	4
1.2	Theses/Dissertations (PhD and HDR)	2
1.3	Book Chapters	19
1.4	Guest Editor for Special Issues of Journals	8
1.5	Journals Articles/Papers	137
1.6	Computer Programs	3
1.7	Articles Disseminating Science to the General Public	3
2.	**Presentations** (In more than 30 countries)	**251**
2.1	Seminars	86
2.2	Conference Presentations (50% invited)	155
2.4	Non-Technical Public Presentations	10
3.	**Conferences & Symposia Organized** (See page 14-16 of this CV for a listing)	**30**

1. Publications

1.1 Books

[4] Cook, R.; Ayers, P. W.; Matta, C. F. (2024). *Electron Localization-Delocalization Matrices*, (*Lecture Notes in Chemistry Series*), Springer – in production/in press. (235 pages).

[3] Matta, C. F.; Huang, L.; Massa, L. (2023). *Quantum Crystallography*, De Gruyter. (215 pages).

[2] Matta, C. F., (Ed.) (2010). *Quantum Biochemistry: Electronic Structure and Biological Activity (Vol. 1 and 2)*, Wiley-VCH, Weinheim. (978 pages).

[1] Matta, C. F.; Boyd, R. J. (Eds.) (2007). *The Quantum Theory of Atoms in Molecules: From Solid State to DNA and Drug Design*, Wiley-VCH, Weinheim, (567 pages).

1.2 Theses / Dissertations

[2] Matta C. F. (2009), *The Response of Molecular Charge Density Distributions to Changes in the External Potential*, HDR Dissertation (Habilitation à diriger des recherches), Université de Lorraine (formerly Univ. Henri Poincaré), Nancy, France (223 pages).

[1] Matta, C. F. (2002), *Applications of the Quantum Theory of Atoms in Molecules to Chemical and Biochemical Problems*, PhD Thesis, McMaster University, Hamilton, Canada. (323 pages).

1.3 Book Chapters

[19] Matta, C. F. (2023). Electron localization-delocalization matrices (LDMs), in: *Comprehensive Computational Chemistry* & *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*, Boyd, R. J.; Yáñez (Eds.), Elsevier, The Netherlands. (pp. 1-13). (Link).

[18] Anderson, J. S. M.; Mortera-Carbonell, A. d.-J.; Matta, C. F. (2023). Non-nuclear maxima in the molecular electron density, Chapter 14 in: *Advances in Quantum Chemical Topology Beyond QTAIM*, Anderson, J. S. M.; Cortés-Guzmán, F.; Rodríguez, J. I. (Eds.), Elsevier, The Netherlands. (pp. 375-388).

[17] Massa, L.; Castanedo, L. A. M.; Fahimi, P.; Matta, C. F. (2023). Applications of in-silico quantum chemical calculations to large systems: The kernel energy method, Chapter 7 in: In-silico *Approaches to Macromolecular Chemistry*, Thomas, M. E.; Thomas, J.; Thomas, S.; Kornweitz, H. (Eds.), Elsevier, The Netherlands. (pp. 199-215).

[16] Massa, L.; Fahimi, P.; Castanedo, L. A. M.; Matta, C. F. (2023) "*In silico approaches and challenges for quantum chemical calculations on macromolecules*", Chapter 6 in: In-silico *Approaches to Macromolecular Chemistry*, Thomas, M. E.; Thomas, J.; Thomas, S.; Kornweitz, H. (Eds.), Elsevier, The Netherlands. (pp. 185-197).

[15] Lombardi, O.; Matta, C. F. (2022). Coarse-graining and the quantum theory of atoms in molecules, Chapter 10 in: *Philosophical Perspectives on Quantum Chemistry*, Lombardi, O.; Martínez González J. C.; Fortin, S. (Eds.), Springer Nature Switzerland AG (pp. 217-241).

[14] Matta, C. F.; Bandrauk, A. D. (2021). An Introduction to laser-fields effects on chemical reactivity, Chapter 11 in: *Effects of Electric Fields on Structure and Reactivity: New Horizons in Chemistry*, Shaik, S; and Stuyver, T. (Eds.), The Royal Society of Chemistry, London (pp. 394-419).

[13] Sowlati-Hashjin, S.; Karttunen, M.; Matta, C. F. (2021). Electrostatic fields in biophysical chemistry, Chapter 7 in: *Effects of Electric Fields on Structure and Reactivity: New Horizons in Chemistry*, Shaik, S; and Stuyver, T. (Eds.), The Royal Society of Chemistry, London (pp. 225-262).

[12] García-Ramos, J. C.; Cortés-Guzmán, F.; Matta, C. F. (2018). On the nature of hydrogen-hydrogen bonding, Chapter 16 in: *Intermolecular Interactions in Molecular Crystals: Fundamentals of Crystal Engineering*, Novoa, J. J. (Ed.), Royal Society of Chemistry, London, UK. (pp. 559-594).

[11] Matta, C. F.; Massa, L. (2017). Information theory and the thermodynamic efficiency of biological sorting systems: Case studies of the kidney and of mitochondrial ATP-synthase,

Chapter 1 in: *Sustained Energy For Enhanced Human Functions and Activity*, Bagchi, D. (Ed.), Academic Press - An imprint of Elsevier, London. (pp. 3-29).

[10] Matta, C. F.; Sumar, I.; Cook, R.; Ayers, P. W. (2016). Localization-delocalization and electron density-weighted connectivity matrices: A bridge between the quantum theory of atoms in molecules and chemical graph theory, Chapter 3 in: *Applications of Topological Methods in Molecular Chemistry* (Springer book series: *Challenges and Advances in Computational Chemistry and Physics* (Vol. 22)), Chauvin, R; Lepetit, C.; Silvi, B.; Alikhani, E. (Eds.), Springer, Switzerland (pp. 53-88).

[9] Matta, C. F. (2010). Reflections on quantum biochemistry: From context to contents, Editorial chapter in: *Quantum Biochemistry: Electronic Structure and Biological Activity (Vol. 1)*, Matta, C. F. (Ed.), Wiley-VCH, Weinheim (pp. XI-L).

[8] Bohórquez, H. J.; Cárdenas, C.; Matta, C. F.; Boyd, R. J.; Patarroyo, M. E. (2010). Methods in biocomputational chemistry: A lesson from the amino acids, Chapter 13 in: *Quantum Biochemistry: Electronic Structure and Biological Activity (Vol. 1)*, Matta, C. F. (Ed.), Wiley-VCH, Weinheim (pp.403-422).

[7] Matta, C. F. (2010). From atoms in amino acids to the genetic code and protein stability, and backwards, Chapter 14 in: *Quantum Biochemistry: Electronic Structure and Biological Activity (Vol. 1)*, Matta, C. F. (Ed.), Wiley-VCH, Weinheim (pp. 423-472).

[6] Arabi, A. A.; Matta, C. F. (2010). Energy richness of ATP in terms of atomic energies: A first step, Chapter 15 in: *Quantum Biochemistry: Electronic Structure and Biological Activity (Vol. 1)*, Matta, C. F. (Ed.), Wiley-VCH, Weinheim (pp. 473-498).

[5] Massa, L.; Matta, C. F.; Yonath, A.,[a] Karle, J.[b] (2010). Quantum transition state for peptide bond formation in the ribosome, Chapter 16 in: *Quantum Biochemistry: Electronic Structure and Biological Activity (Vol. 2)*, Matta, C. F. (Ed.), Wiley-VCH, Weinheim (pp. 501-516).

[4] Matta, C. F.; Boyd, R. J. (2007). Introduction to the quantum theory of atoms in molecules, Chapter 1 in: *Quantum Theory of Atoms in Molecules: From Solid State to DNA and Drug Design*, Matta, C. F. and Boyd, R. J. (Eds.), Wiley-VCH, pp.1-34.

[3] Matta, C. F. (2006). Hydrogen-hydrogen bonding: The non-electrostatic limit of closed-shell interaction between two hydrogen atoms. A critical review, Chapter 9 in: *Hydrogen Bonding - New Insight*, (*Challenges and Advances in Computational Chemistry and Physics Series*), Grabowski S. (Ed.), Springer, pp. 337-375.

[2] Matta C. F. (2005). Computational chemistry: A powerful and inexpensive tool for basic and applied research in the life sciences, Chapter 23 in: *Discovery to Delivery: BioVision Alexandria 2004* (*Proceedings of the World Biological Forum)*, Serageldin, I. and Persley, G. J. (Eds.), CABI Publishing, pp. 261-272.

[1] Bader, R. F. W.; Matta, C. F.; and Martín, F. J. (2003). Atoms in medicinal chemistry, Chapter 7 in: *Medicinal Quantum Chemistry* (*Methods and Principles in Medicinal Chemistry Series*), Alber, F. and Carloni, P. (Eds.), Wiley-VCH, Weinheim, pp. 201-232.

[a] Nobel Laureate (Chemistry, 2009).
[b] Nobel Laureate (Chemistry, 1985).

1.4 Guest Editor for Special Issues of Journals & Themed Collections

[8] **Guest Editors:** Brovarets, O. O.; Hovorun, D. M.; Matta, C. F.; Pérez-Sanchez, H. (2020). Themed Article Collection: "Proton Transfer Processes in Biological Reactions: A Computational Approach" *Frontiers in Chemistry* (DOI: 10.13140/RG.2.2.21042.45765). (7 articles by 33 authors).

[7] **Guest Editors:** Matta, C. F.; Hutter, M. (2018). "*Special Focus Issue: Computational Chemistry*" *Future Medicinal Chemistry,* Volume **10**, Issue 13 (July 2018), pp. 1517-1635. (12 articles by 34 authors).

[6] **Guest Editors:** Matta, C. F.; Massa, L. (2018). "*Special Issue: Quantum Crystallography - PART 2 of 2*" *Journal of Computational Chemistry,* Volume **39**, Issue 18 (5 July 2018), pp. i, 1077-1167. (8 articles by 27 authors).

[5] **Guest Editors:** Matta, C. F.; Massa, L. (2018). "*Special Issue: Quantum Crystallography – PART 1 of 2 "* *Journal of Computational Chemistry,* Volume **39**, Issue 17 (30 June 2018), pp. i, 1013-1075. (8 articles by 11 last article by Professor Robert G. Parr published posthumously).

[4] **Guest Editor:** Matta, C. F. (2017). "*Special Issue: Honoring Professor Lou Massa - A Path through Quantum Crystallography*" *Structural Chemistry,* Volume **28**, Issue 5 (October 2017), pp. 1277-1605 (33 articles by 84 authors including an article by Nobel Laureate Ada Yonath).[a] (Link)

[3] **Guest Editor:** Matta, C. F. (2014). "*Special Issue (Part 2 of 2): Philosophical Aspects and Implications of the Quantum Theory of Atoms in Molecules*" *Foundations of Chemistry,* Volume **16**, Issue 1 (April 2014), pp. 1-84 (4 articles). (Link)

[2] **Guest Editor:** Matta, C. F. (2013). "*Special Issue (Part 1 of 2): Philosophical Aspects and Implications of the Quantum Theory of Atoms in Molecules*" *Foundations of Chemistry,* Volume **15**, Issue 3 (October 2013), pp.243-341 (8 articles). (Link)

[1] **Guest Editor:** Matta, C. F. (2011). "*Professor Richard F. W. Bader Festschrift"* *The Journal of Physical Chemistry A* Vol. **115**, No. 54 (17 November 2011), pp. 12427-13209 (80 articles by 450 authors). (Link)

1.5 Journals Articles / Papers

[137] **Hooft, G.;**[b] **Phillips, W. D.;**[c] **Zeilinger, A.;**[d] Allen, R. A.; Baggott, J.; Bouchet, F.; Cantanhede, S. M. G.; **Castanedo, L. A. M. [MY PhD STUDENT]**; Cetto, A. M.; Coley, A. C.; Dalton, B. J.; **Fahimi, P. [MY PhD STUDENT]**; Franks, S.; Frano, A.; Fry, E. S.; Goldfrab, S.; Langanke, K.; Nanopoulos, D.; **Matta, C. F.;** Orzel, C.; Patrick, S.; Sanghai, V. A. A.; Shpyrko, O.; Schuller, I. K.; Lidstrom, S. (2023). "The sounds of science - a symphony for many instruments, and voices - Part II", *Physica Scripta*, minor changes requested before acceptance (revised version submitted). **[Invited to co-author this paper with some of the**

[a] Five more papers by 18 additional authors were submitted to this issue but ended-up in other issues of *Structural Chemistry*.
[b] Nobel Laureate (Physics, 1999).
[c] Nobel Laureate (Physics, 1997).
[d] Nobel Laureate (Physics, 2022).

world foremost physicists].

[136] Naghdian, N.; Ahadib, Z.; Davoodia, J.; Matta, C. F.; Shadman, M. (2023). "Electrodialysis desalination: Borophene membrane for ion separation using non-equilibrium molecular dynamics"; *Journal of Molecular Liquids*, major revisions requested (in revision).

[135] Gaser, O. A.; Nasr, M. A.; Hussein, A. E.; Salah, R. A.; Saad, S. M.; Abd Elmourdy, N.; Elmehrath, A. O.; Ehab, S.; Salah, A., Chang, Y.-T.; Hedrick, M.; Castanedo, L. A. M.; Fahimi, P.; **Matta, C. F.**; El Badri, N. (2023). "Mitochondrial temperature as a biomarker for hepatocellular carcinoma", *Advanced Biology*, submitted, in review.

[134] Azzouz, L.; Rérat, M.; Matta, C. F. (2023). "Tuning novel $NaLaS_{2(1-x)}$(Se or Te)$_{2x}$ alloys as light-absorbing materials by dopant-induced crystallographic phase and electronic structure transitions", *Journal of Physical Chemistry C* **127**, 17532−17544. **[Journal cover feature article]**.

[133] Fahimi, P.; Matta, C. F.; Okie, J. G. (2023). "Are size and mitochondrial power of cells inter-determined?"; *Journal of Theoretical Biology* **572**, Article # 111565 (pp.1-12).

[132] Taheri, S.; Ahadi, Z.; Matta, C. F.; Ghanbarzadeh, S.; Lakmehsari, M. S. (2023). "The effects of the nature of the sterol on the properties and stability of niosome bilayer vesicles"; *Journal of Molecular Liquids* **369**, Article # 120811 (pp. 1-27).

[131] Castanedo, L. A. M.; Matta, C. F. (2022). "On the Prebiotic Selection of Nucleotide Anomers: A Computational Study"; *Heliyon* 8, e09657 (pp. 1-12).

[130] Castanedo, L. A. M.; Matta, C. F. (2022). "On the Prebiotic Selection of Nucleotide Anomers: Computational Data"; *Mendeley Data* **V2**, DOI: 10.17632/khxvtshbs2.2.

[129] Jara-Cortés, J.; Matta, C. F.; Hernández-Trujillo, J. (2022). "A Fast Approximate Extension of the Interacting Quantum Atoms Energy Decomposition to Excited States"; *Journal of Computational Chemistry* **43**, 1068-1078.

[128] Smith, E. R.; Smith, F.; Harriott, T. A.; Majaess, D.; Massa, L.; Matta, C. F. (2022) "Novel correlations between diffuse interstellar bands and optical reddening"; *Research Notes of the American Astronomical Society (RNAAS)* **6** (No. 4), 82.

[127] Vigneau, J.-N.; Fahimi, P., Ebert, M.; Cheng, Y.; Tannahill, C.; Muir, P.; Nguyen-Dang, T.-T. Matta, C. F. (2022). "ATP synthase: A moonlighting enzyme with unprecedented functions", *Chemical Communications (ChemComm)* **58**, 2650-2653. [**Cover Feature**].

[**NEWS item in:** Apps, S. "Electric field of ATP synthase suggests enzyme has functions beyond catalysis" *Chemistry World* (28 Feb. 2022)]

[126] Lakmehsari, M. S.; Yeganegi, S.; Matta, C. F.; Ghandi, K.; Ziaie, F. (2022). "The diffusion of light gases through polyvinyl butyral: Molecular hydrogen, helium, and neon"; *Journal of Molecular Liquids* **345**, Article # 118245 (pp. 1-7).

[125] Azzouz, L.; Halit, M.; Denawi, H.; Charifi, Z.; Baaziz, H.; Rérat, M.; Matta, C. F. (2022). "$RbCeX_2$ Crystal (X = S, Se, Te): Pressure-induced spin-selective gapless transition and response properties", *Journal of Alloys and Compounds* **898**, Article # 162760, (pp. 1-12).

[124] Castanedo, L. A. M.; Matta, C. F.; Ylijoki, K. E. O. (2022). "The reaction path of cyclooctatetraene dimerization revisited"; *International Journal of Quantum Chemistry*

122, Article # e26866, (pp. 1-16).

[123] Fahimi, P.; Matta, C. F. (2022). "The hot mitochondrion paradox: Reconciling theory and experiment"; *Trends in Chemistry* **4**, 96-110. [Selected for **"two-months free access"** by the Editor].

[122] Matta, C. F.; Massa, L. (2022). "A two projector triple product in quantum crystallography"; *International Journal of Quantum Chemistry* **122**, Article # e26838 (1-7). **[Cover Feature].**

[121] Matta, C. F.; Huang, L.; Massa, L. (2022). "Quantum crystallography: *N*-representability big and small"; *Israel Journal of Chemistry* **62**, 159-171 (Article # e202100108). [**Invited**].

[120] Smith, F.; Majaess, D.; Harriott, T. A.; Massa, L.; Matta, C. F. (2021) "Establishing new diffuse interstellar band correlations to identify common carriers"; *Monthly Notices of the Royal Astronomical Society (MNRAS)* **507**, 5236–5245.

[119] Anderson, J. S. M.; Massa, L.; Matta, C. F. (2021). "Non-nuclear maxima and the universality of Bright Wilson's justification of the first Hohenberg Kohn theorem revisited"; *Chemical Physics Letters* **780**, Article # 138940, pp. 1-6. [**"Editor's Choice"** and **"Cover Feature"**].

[118] Fahimi, P.; Matta, C. F. (2021). "On the Power per Mitochondrion and the Number of Associated Active ATP Synthases"; *Physical Biology* **18**, Article # 04LT01, pp. 1-6.

[117] Fahimi, P.; Toussi, C. A.; Trump, W.; Haddadnia, J.; Matta, C. F. (2021). "Striking patterns in natural magic squares' associated electrostatic potentials: Matrices of the 4th and 5th order", *Discrete Mathematics* **344**, Article # 112229, pp. 1-11.

[116] Sadjadi, SA; Matta, C. F.; Hamilton, I. P. (2021). "Bonding and metastability for group 12 dications", *Journal of Computational Chemistry* **42**, 40-49.

[115] Toussi, C. A.; Haddadnia, J.; Matta, C. F. (2021). "Drug design by machine-trained elastic networks. Predicting Ser/Thr-protein kinase inhibitors' activities", *Molecular Diversity* **25**, 899-909.

[114] Sowlati-Hashjin, S.; Karttunen, M.; Matta, C. F. (2020). "Manipulation of diatomic molecules with oriented external electric fields: Linear correlations in atomic properties lead to non-linear molecular responses", *Journal of Physical Chemistry A* **124**, 4720-4731. [**Supplementary Cover Feature**]

[113] Janbazi, M.; Azar, Y. T.; Ziaie, F.; Ghandi, K.; Matta, C. F.; Lakmehsari, M. S. (2020) "Structures, g-tensors, and hyperfine coupling constants of L-α-alanine radicals in radiation dosimetry: An *ab initio* molecular dynamics simulation"; *International Journal of Quantum Chemistry* **120** (issue 12), Article # e26211, pp. 1-13.

[112] Fahimi, P.; Nasr, M. A.; Castanedo, L. A. M.; Cheng, Y.; Toussi, C. A.; Matta, C. F. (2020). "Invited paper (mini review): A note on the consequences of a hot mitochondrion: Some recent developments and open questions"; *Biophysical Bulletin* **Iss. 43**, 14-21. **[Invited Paper]**.

[111] Matta, C. F.; Lombardi, O.; Arriaga, J. J. (2020). "Two-step emergence: The quantum theory of atoms in molecules as a bridge between quantum mechanics and molecular chemistry", *Foundations of Chemistry* **22**, 107-129.

[110] Kandezi, M. K.; Lakmehsari, M. S.; Matta, C. F. (2020). "Electric field assisted desalination of water using B- and N-doped-graphene sheets: A non-equilibrium molecular dynamics study", *Journal of Molecular Liquids* **302**, Article#112574, pp. 1-10.

[109] Azzouz, L.; Halit, M.; Charifi, Z.; Baaziz, H.; Rérat, M.; Denawi, H.; Matta, C. F. (2020). "Magnetic semiconductor properties of $RbLnSe_2$ (Ln = Ce, Pr, Nd, Gd): A density functional study", *Journal of Magnetism and Magnetic Materials* **501**, Article# 166448 (pp.1-8).

[108] Castanedo, L. A. M.; Lamar, A. S.; Boado, C. M.; de la Nuez Veulens, A.; Matta, C. F. (2019). "Genoprotection by Complexation: The Case of *Phyllanthus orbicularis* K extract", *Computational and Theoretical Chemistry* **1164**, 112555, pp. 1-9.

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[3] Matta, C. F. (2023). « Sur la transdisciplinaité de la théorie des graphes et des réseaux » [On the transdisciplinarity of graph and networks theory], Actes du colloque *ACFAS Transdisciplinarité et évolution des savoirs : fondements et pratiques* qui a eu lieu à Montréal le 11-12 mai 2023.

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[1] Matta, C. F. ; Koch, D. ; Roy, P.-N. ; Peslherbe, G. (2019). "La chimie théorique en langues latines ou faire de la science dans sa langue maternelle" [Theoretical chemistry in Latin languages or doing science in one's mother tongue]; *Découvrir (Acfas magazine)*; Tribue published online 16 October 2019 (https://www.acfas.ca/node/53351).

2. Presentations

2.1 Seminars

86 Seminar: Department of Chemistry, *Université de Sherbrooke*, Sherbrooke, Québec, (Canada), "L'ATP Synthase : Plus qu'un simple biocatalyseur ?", (8 November 2023). (Host: Prof. Jérôme Claverie).

85 Invited Guest Lecturer in the Graduate Course "Computational Sciences and Artificial Intelligence in Medicinal applications": Department of Biochemistry, *United Arab Emirates University*, Abu Dhabi, (United Arab Emirates), "ATP Synthase Beyond Catalysis", (18

October 2023). (Host: Prof. Alya A. Arabi).

84 Seminar: Faculty of Chemistry & Biological and Chemical Research Centre, *University of Warsaw*, Warsaw, (Poland), "ATP Synthase Beyond Catalysis", (27 September 2023). (Host: Prof. Dr. Habil. Krzysztof Woźniak & Prof. Dr. Habil. Paulina Dominiak).

83 Seminar: Department of Chemistry, *University of Pretoria*, Pretoria, (South Africa), "ATP Synthase Beyond Catalysis", (13 December 2022). (Host: Prof. Ignacy Cukrowski).

82 Seminar: School of Chemistry, *University of the Witwatersrand*, Johannesburg, (South Africa), "ATP Synthase Beyond Catalysis", (12 December 2022). (Host: Prof. Ignacy Cukrowski).

81 Seminar: Computational Chemistry & Chemoinformatics Drug Discovery Program, *Ontario Institute for Cancer Research*, Toronto, ON (Canada), "ATP Synthase Beyond Catalysis: Novel Functions in Metabolism Stemming from its very Structure", (26 July 2022). (Host: Dr. Gennady Poda, Scientific Advisor & Group Leader).

80 Seminar: Department of Chemistry, *Simon Fraser University*, Vancouver, BC (Canada), "ATP Synthase Beyond Catalysis: Novel Functions in Metabolism Stemming from its very Structure", (6 July 2022). (Host: Prof. Vance Williams).

79 *Atlantic Science Tour Seminar:* Départment de Chimie, *Université de Moncton*, Moncton, NB (Canada), "L' ATP synthase : une machine, une enzymes et plus encore. Peut-être bien plus !", (1 April 2022). (Host: Prof. Luc Tremblay).

78 *Atlantic Science Tour Seminar:* Department of Chemistry, *Saint Francis Xavier University*, Antigonish, NS (Canada), "ATP synthase: An enzyme machine and more. Perhaps much more!", (25 March 2022). (Host: Prof. Erwan Bertin).

77 *Atlantic Science Tour Seminar:* Department of Chemistry, *University of New Brunswick*, Fredericton, NB (Canada), "ATP synthase: An enzyme machine and more. Perhaps much more!", (28 Jan. 2022). (Host: Professor Stijn De Baerdemacker).

76 *Atlantic Science Tour Seminar:* Department of Chemistry, *Mount Allison University*, Sackville, NB (Canada), "ATP synthase: An enzyme machine and more. Perhaps much more!", (17 Jan. 2021). (Host: Professor Megan. G Roberts).

75 Seminar: Helmy Institute for Medical Sciences (HIMS), *Zewail City of Science and Technology*, 6th October City, Guiza (Egypt), "ATP synthase: An enzyme machine and more. Perhaps much more!", (8 Dec. 2021). (Host: Professor Nagwa El Badri).

74 *Atlantic Science Tour Seminar:* Department of Chemistry, *Acadia University*, Wolfville, NS (Canada), "ATP synthase: An enzyme machine and more. Perhaps much more!", (4 Nov. 2021). (Host: Professor Vlad Zamlynny).

73 *Atlantic Science Tour Seminar:* Department of Chemistry, *Memorial University of Newfoundland*, St. John's, NL (Canada), "ATP synthase: An enzyme machine and more. Perhaps much more!", (26 Oct. 2021). (Host: Professor Kark Jobst).

72 *Atlantic Science Tour Seminar:* Department of Chemistry, *Cape Breton University*, Syndey, NS (Canada), "ATP synthase: An enzyme machine and more. Perhaps much more!", (21 Oct. 2021). (Host: Professor Stephanie MacQuarrie). [Delivered remotely].

71. Joint Chemistry and Biology Seminar: Faculty of Arts and Science, *Concordia University*, Montreal (Canada), "Electrical and Thermal Control in the Mitochondrion", (31 January 2020). (Host: Professor Gilles Peselherbe).

70. Seminar: Facultad de Ciencias, *Universidad de la República*, Montevideo, (Uruguay), "Riñones, mitocondrias, y el demonio de Maxwell: sobre la eficiencia de las máquinas de clasificación biológica" delivered in Spanish [Kidneys, Mitochondria, and Maxwell's Demon: On the Efficiency of Biological Sorting Machines], (17 May 2019). (Host: Prof. E. Laura Coitiño).

69. Seminar: Dept. of Physics and Atmospheric Science, *Dalhousie University*, Halifax, NS (Canada), "Kidneys, Mitochondria, and Maxwell's Demon: On the Efficiency of Biological Sorting Machines", (30 November 2018). (Host: Prof. Jesse Maassen).

68. Seminar: Institute of High Technologies, *Taras Shevchenko National University*, Kiev (Ukraine), "Molecules as Networks of Electron Localization and Delocalization". (9 Nov. 2018). (Hosts: Prof. Volodymyr Ilchenko and Prof. Dmytro M. Hovorun).

67. Seminar: Institute of Physics, *National Academy of Sciences of Ukraine*, Kiev (Ukraine), "Molecules as Networks of Electron Localization and Delocalization". (9 Nov. 2018). (Secretary of the Seminar: S. O.Esylevskyy, Host: Prof. Galina Dovbeshko).

66. Seminar: Institute of Physics, *National Academy of Sciences of Ukraine*, Kiev (Ukraine), "Kidneys, Mitochondria and Maxwell's Demon: An Information Theoretical Investigation". (9 Nov. 2018). (Secretary of the Seminar: S. O.Esylevskyy, Host: Prof. Galina Dovbeshko).

65. Seminar: Institute of High Technologies, *Taras Shevchenko National University*, Kiev (Ukraine), "The Kidney, the Mitochondrion, and Maxwell's Demon – An Information Theoretic Investigation of Molecular Motors Thermodynamic Efficiency". (7 Nov. 2018). (Hosts: Prof. Volodymyr Ilchenko and Prof. Dmytro M. Hovorun).

64. Zewail City's President Lecture Series: Helmy Institute for Medical Sciences (HIMS), *Zewail City of Science and Technology*, 6th of October City, Giza (Egypt), "Kidneys, Mitochondria, and Maxwell's Demon: An Information Theory Investigation", (28 August 2018). (Host: Professor Nagwa El-Badri, Director of the Institute).

63. Seminar: *The Rugjer Bošković Institute*, Zagreb, Croatia, "Molecules as Networks: An Electron Localization-Delocalization Matrices Approach", (23 July 2018). (Host: Dr. Sonja Nicolić).

62. Group Research Seminar: Dept. of Chemistry, *Oregon State University* (Corvalis, Oregon, USA), "Molecules as Networks". (8 May 2018). (Host: Prof. Paul Ha-Yeon Cheong).

61. Seminar [in Spanish]: Dept. of Chemistry, *Oviedo University* (Spain), "Moléculas como redes de localización y de deslocalización de electrones". (Molecules as Networks of Electron Localization and Delocalization). (7 November 2017). (Host: Prof. Ángel Martín Pendás).

60. Special Seminar: Dept. of Chemistry, Hunter College, *City University of New York (CUNY)*, NY, NY (USA), "Molecules as a Networks: Electron Delocalization Channels as a Novel Predictive Tool for Structure-Activity Relationships." (24 May 2017). (Host: Prof. Charles Mike Drain).

59. Seminar: Dept. of Chemistry, *York University*, Toronto (Canada), The Electron Localization-Delocalization Matrix (LDM): A Novel, Compact, and Powerful Molecular Descriptor. (23 March 2017). (Host: Prof. René Fournier).

58. Seminar: Dept. of Chemistry, *The Hebrew University of Jerusalem*, Jerusalem (Israel), "Localization-Delocalization Matrices (LDMs): A Powerful Molecular Descriptor for Quantitative Structure Activity Relationships (QSARs)". (7 December 2016). (Host: Prof. Sason Shaik).

57. Seminar: Unité de recherche Matériaux Nouveaux et Dispositifs Électroniques (UR 11ES55), Faculté des Science, *Université de Monastir*, Monastir (Tunisia), "Les matrices de localisation et de délocalisation d'électrons (LDMs): une description utile et compacte du graphe moléculaire flou" (In French) (Electron Localization and Delocalization Matrices (LDM)s: A Useful and Compact description of the Fuzzy Molecular Graph). (3 October 2016). (Hosts: Dr. Ayachi Sahbi and Prof. Moncef Msadek).

56. Seminar: Dept. of Chemistry, *Mount Allison University*, Sackville, NB, (Canada), "The Electron Localization-Delocalization Matrix (LDM): A New and Far-Reaching Molecular Fingerprinting Tool". (8 April 2016). (Host: Prof. Khashayar Ghandi).

55. Seminar: Dept. of Chemistry, *Dalhousie University*, Halifax, NS, (Canada), " Localization-Delocalization Matrices (LDMs): A Bridge between Chemical Graph Theory and the Quantum Theory of Atoms in Molecules". (18 March 2016). (Host: Prof. Erin Johnson).

54. Seminar: Dept. of Chemistry, *Université Laval*, Québec (Canada), "Les matrices de localisation et de délocalisation d'électrons (LDMs): un pont entre la théorie chimique des graphes et la théorie quantique des atomes dans les molécules". (11 March 2016). (Host: Prof. Anna Richey).

53. Seminar: School of Pharmacy, *The Hebrew University of Jerusalem*, Jerusalem (Israel), "Molecular Fingerprinting from the Electron Density and Electron Localization-Delocalization Descriptors in Quantitative Structure-to-Activity Relationships (QSAR)". (2 Sept. 2015). (Host: Prof. Amiram Goldblum).

52. Seminar: Dept. of Structural Biology, *Weizmann Institute of Science*, Rehovot (Israel), "Some Aspects of External Electric Field-Effects on Small Molecules and their Reactivity". (25 August 2015). (Host: Prof. Ada Yonath **([a])**, Director of the Institute).

51. Official Seminar: *Max Planck Institute for Chemical Physics of Solids*, Dresden (Germany), "What Happens to Chemical Bonding upon Beta-Decay Nuclear Transmutation". (6 August 2015). (Host: Prof. Dr. Juri Grin, Director of the Institute, and Dr. Miroslav Kohout - Senior Scientist).

50. Special Topics in Theoretical Chemistry Seminar: *Swiss Federal Institute of Technology (ETH–Zürich)*, Zürich, Switzerland, "Electron Localization-Delocalization Matrices: Some Recent Applications". (4 August 2015). (Host: Prof. Dr. Markus Reiher).

49. Seminar [in Spanish]: Dept. of Chemistry, *Oviedo University* (Spain), "Las matrices de localización y deslocalización (LDMs): Una fusión de la Teoría Química de los Grafos (CGT) y la Teoría de los Átomos en Moléculas de Bader (QTAIM)" (In Spanish: Localization and

[a] Nobel Laureate in Chemistry (2009).

Delocalization Matrices: A Fusion of Chemical Graph Theory and Bader's Theory of Atoms in Molecules). (2 June 2015). (Host: Prof. Ángel Martín Pendás).

48. Seminar: Dept. of Chemistry, *Saint Mary's University* (Halifax, Canada), "The Localization-Delocalization Matrix: A Compact Descriptor of the Whereabouts of Electrons and its Correlation with Experiment". (21 Nov. 2014). (Host: Prof. Jason Clyburne).

47. Seminar: Gas Processing Center (GPC), College of Engineering, *Qatar University* (Doha, Qatar), "Modeling Biophysical and Biological Properties from the Characteristics of the Molecular Electron Density and the Electron Localization-Delocalization Matrices (LDMs)". (16 June 2014). (Host: Dr. Mohamed Shibl).

46. Seminar: Dept. of Physics & Dept. of Chemistry, *The Hong Kong University* (Hong Kong), "The Evolution of Chemical Bonding over the Nuclear Transmutation Reaction Path" (13 June 2014). (Hosts: Prof. S. Kwok and Dr. SeyedAbdolreza Sadjadi).

45. "Guest-Lecture of the Chair or Chemical Physics and Materials Science": *Institut für Physik, Universität Augsburg*, Augsburg (Germany). "Some Aspects of Molecular Response to External Electric Fields", (12 Nov. 2013). (Host: Prof. Dr. Wolfgang Scherer).

44. Guest Lecturer [in Spanish]: 2 hours class of 2nd year Quantum Chemistry I (1404), *School of Chemistry*, *Universidad Nacional Autónoma de México (UNAM)*, "Electric field effects on molecular systems", (18 Oct. 2013). (Host: Prof. Jesus Hernandez-Trujillo).

43. Seminar [in Spanish]: *El Instituto Mexicano del Petróleo (IMP)* (*Mexican Institute for Petroleum*), "The chemical bond under external electric fields: A computational study", (16 Oct. 2013). (Host: Dr. Isidoro García-Cruz).

42. Seminar [in Spanish]: *Dept. of Chemistry, Cinvestav, Centro de Investigación y de Estudios Avanzados del I.P.N.*, México D. F. (*National Center for Advanced Studies - Mexico*), "Computational investigations of electric field-effects on chemical bonding, electron density, and reactivity", (14 Oct. 2013). (Host: Prof. Alberto Vela).

41. Seminar: *Dept. of Chemistry, New York University,* New York. "Computational Explorations of Intense Electric Field-Effects on Reaction Paths", (6 March 2013). (Host: Prof. Nicholas E. Geacintov).

40. Guest Speaker - *Competence Center for Computational Chemistry* (**C4**) *Seminar Programme* co-organized by ETH−Zürich, the University of Zürich, IBM Research, and EPFL: *Swiss Federal Institute of Technology (ETH−Zürich)*, Zürich, Switzerland "The Continuum of Hydrogen-Hydrogen Interactions in Molecules and Crystals", (26 May 2011). (Hosts at ETH: Profs. Markus Reiher & Hans Peter Luthi).

39. Guest Speaker - *Competence Center for Computational Chemistry* (**C4**) *Seminar Programme* co-organized by ETH−Zürich, the University of Zürich, IBM Research, and EPFL: *École Polytechnique Féderale de Lausanne (EPFL)*, Lausanne, Switzerland, "The Continuum of Hydrogen-Hydrogen Interactions in Molecules and Crystals", (25 May 2011). (Hosts at EPFL: Profs. Ursula Röthlisberger & Clémence Corminboeuf).

38. Seminar: *Dept. of Chemistry, Université de Sherbrooke (Sherbrooke, QC, Canada).* "Hydrogen-Hydrogen Bonding: A Weak Interaction in Molecules and Crystals" (23 Feb. 2011). (Host: Prof. André Bandrauk).

37. Seminar: *Dept. of Chemistry, Hunter College, City University of New York (CUNY),* "The Stabilizing Nature of the Ubiquitous Hydrogen-Hydrogen (H...H) Close Contacts: Should the Texbook Concept of H...H Steric Repulsion be Revisited?", (12 Nov. 2010). (Host: Prof. Lou Massa).

36. Seminar [in Arabic]: *Department of Spectroscopy, National Research Centre (NRC)*, Cairo, Egypt, "The Stabilizing Nature of the Ubiquitous Hydrogen-Hydrogen (H...H) Close Contacts: Should the Textbook Concept of H...H Steric Repulsion be Revisited?", 30 Aug. 2010 (Host: Prof. Medhat A. A. Ibrahim).

35. Seminar: *Center for Computational Materials Science*, *United States Naval Research Laboratory* (NRL), Washington DC, "Hydrogen-Hydrogen Bonding: A Stabilizing Interaction in Molecules and Crystals", (23 July 2010). (Host: Dr. Lulu Huang).

34. Seminar: *The Rugjer Bošković Institute*, Zagreb, Croatia, "H-H Bonding in Molecules and Crystals: A Stabilizing Interaction not a 'Steric Clash'", (14 June 2010). (Hosts: Prof. Nenad Trinajstić & Dr. Sonja Nicolić).

33. Seminar: *The Rugjer Bošković Institute*, Zagreb, Croatia, "Where do Things Happen in Biological Molecules? Clues from the Topology of the Electron Density", (16 July 2009). (Hosts: Prof. Nenad Trinajstić & Dr. Sonja Nicolić).

32. Joint seminar: *Institute of Biomolecular Chemistry* & *Institute of Structural Chemistry, Hungarian Academy of Sciences*, Budapest, Hungary, "Where do Things Happen in Biological Molecules? Clues from the Topology of the Electron Density", (19 June 2009). (Hosts: Profs. György Hajós & János Mink).

31. Seminar: *Departamento de Física y Química Teórica, Facultad de Química, Universidad Nacional Autónoma de México (UNAM), México D. F.,* "Hydrogen-Hydrogen Bonding: A Non-Electrostatic Interaction between Hydrogen Atoms in Molecules", (6 Aug. 2008). (Host: Prof. Jesús Hernández-Trujillo).

30. Seminar: *Departamento de Quimica Fisica y Analitica, Universidad de Oviedo, Spain*. "A QTAIM Study of DNA Bases", (11 July 2008). (Host: Prof. Angel Martin-Pendas).

29. Seminar [in Arabic]: *Dept. of Biophysics, Cairo University,* "Electron Density of Biomolecules PART 2: Ionization", (25 May 2008). (Host: Prof. Osiris Girgis).

28. Seminar [in Arabic]: *Dept. of Biophysics, Cairo University,* "Electron Density of Biomolecules PART 1: Bond Making and Breaking", (19 May 2008). (Host: Prof. Osiris Girgis).

27. Seminar: *Dept. of Chemistry, Saint Mary's University* "Bond Making and Breaking: From ATP to the Active Site of the Ribosome", (15 February 2008).

26. "Faculty Dialogue Series Presentation": *Research and International Office, Mount Saint Vincent University's* "Dancing with Electrons: Where is Chemistry in all that Jazz? (An Informal Presentation)", (16 November 2007).

25. Seminar: *Department of Biochemistry & Molecular Biology, Dalhousie University (Halifax, Canada)*, "Where Do Things Happen in Biological Molecules? Insight from the Analysis of Molecular Electron Density Distributions", (25 October 2007). (Host: Prof. Jan Reiney).

24. Seminar [in Arabic]: *Faculty of Pharmacy, Alexandria University, (Alexandria, Egypt).*

*"*Quantum Chemical Calculations in Drug Design", (28 Aug. 2007). (Host: Prof. Ibrahim Labouta).

23. Seminar [in French]: *Laboratoire de Chimie de Coordination, Centre national de la recherche scientifique (CNRS), (Toulouse, France).* La théorie quantique des atomes dans les molécules de Bader (QTAIM) : les énergies atomiques et la dissociation des liaisons chimiques, (13 July 2007). (Host: Dr. Noël Lugan)

22. Seminar [in French]: *Laboratoire de Cristallographie et Modelisation des Matériaux Minéraux et Biologiques (LCM3B), Univérsité Henri Poincaré & Centre national de la recherche scientifique (CNRS), (Nancy, France).* "Bond Dissociation: Insight from the Theory of Atoms in Molecules", (22 June 2007). (Host: Prof. Claude Lecomte).

21. Seminar [in French]: *LCM3B, Univérsité Henri Poincaré & CNRS, (Nancy, France).* "The Stabilizing Hydrogen-Hydrogen Closed-Shell Interaction: Fiction or Reality?", (25 May 2007). (Host: Prof. Claude Lecomte).

20. Seminar: *Dept. of Chemistry, Université de Sherbrooke (Sherbrooke, QC, Canada).* "Bond Dissociation: Insight from the Theory of Atoms in Molecules, (2 May 2007). (Host: Prof. André Bandrauk).

19. Seminar [in Arabic]: *Faculty of Pharmacy*, *Alexandria University*, (Alexandria, Egypt), "The Electron Density in Drug Research", (26 February, 2007). (Host: Prof. Labiba K. El-Khordagui).

18. Seminar: *Dept. of Chemistry, Dalhousie University (Halifax, NS, Canada).* "Where Do Things Happen in a Molecule? From Local Properties to Chemical Bonding and Reactivity", (20 March 2006). (Host: Prof. Russell Boyd).

17. Seminar: *Dept. of Chemistry & Physics, Mount Saint Vincent University (Halifax, NS, Canada).* "Where Do Things Happen in a Molecule? From Local Properties to Chemical Bonding and Reactivity", (13 March 2006). (Host: Prof. Katherine Darvesh).

16. Seminar: *Chemical Computing Group (CCG), Inc. (Montréal, QC, Canada).* "Electron density-based quantitative structure-to-property relationships: An emerging line of research", (19 March 2004).

15. Seminar [in Arabic]: *Dept. of Bioscience & Technology, Institute of Graduate Studies and Research, Alexandria University (Alexandria, Egypt).* "Some biophysical and biochemical applications of molecular electron density analysis", (12 January 2004). (Hosts: Profs. Mohammed El-Raey & Taha Zaghlool).

14. Seminar [in Arabic]: *Dept. of Chemistry, Faculty of Science, Alexandria University (Alexandria, Egypt).* "The electron density: A tool for rationalizing bonding and reactivity", (5 January 2004). (Host: Prof. Adel Naguib Assaad).

13. Seminar: *ArQule, Inc. (Woburn, Massachusetts, USA).* "Electron Density-Based Drug Design: An Emerging Line of Research", (26 September 2004).

12. Guest Lecturer: Biological Chemistry CHM447 (4th year), *Department of Chemistry, University of Toronto*. "Computational Chemistry and Enzymes", (12 Feb. 2004). (Host: Prof. Deborah Zamble).

11. Seminar [in French]: *Dept. of Chemistry, Université de Sherbrooke (Sherbrooke, QC, Canada).* "Les relations structure-propriété basées sur la densité électronique: l'interaction entre la théorie et l'expérimentation", (24 Sept. 2003). (Host: Prof. André Bandrauk).

10. "Official Seminar, Chemistry": *Università di Milano (Milan, Italy*). "Some Aspects of Bonding in Aromatic Hydrocarbons", (15 September 2003). (Host: Dr. Carlo Gatti, National Research Center of Italy - CNR).

9. Seminar: *Dept. of Chemistry, Hunter College, City University of New York (CUNY), (New York, NY, USA).* Seminar, "The Electron Density of the Amino Acids and their Experimental Physico- Chemical Properties", (16 June 2003). (Host: Prof. Lou Massa).

8. Graduate Department of Pharmaceutical Sciences Seminar: *Leslie Dan Faculty of Pharmacy, University of Toronto (Toronto, ON, Canada)*. "An Atoms-in-Molecules Study of the Electron Density Distributions of the Amino Acids: Implications on Protein Stability, Molecular Recognition, and Genetic Coding", (2 May 2003). (Host: Prof. Tigran Chalikian).

7. Physical Chemistry Departmental Seminar: *Dept. of Chemistry, University of Toronto (Toronto, ON, Canada).* "The Electron Density of the Genetically-Encoded Amino Acids and of certain H-H Bonded Systems", (11 March 2003). (Host: Prof. Cynthia Gho).

6. Seminar: *Dept. of Chemistry, Dalhousie University (Nova Scotia, NS, Canada).* "The Electron Density of the Genetically-Encoded Amino Acids and of certain H-H Bonded Systems", (14 Feb. 2003). (Host: Prof. Russell Boyd).

5. Seminar: *Chemistry Department, University of Toledo (Toledo, Ohio, USA).* "AIM Study of the Genetically-Encoded Amino Acids: Focus on Correlation with Experiment", (29 Jan. 2003). (Host: Prof. Alan Pinkerton).

4. Guest Lecturer: Quantum Chemistry and Spectroscopy Course, 4th year - *Department of Chemistry, University of Toronto*. "Chemical and Biochemical Applications of the Quantum Theory of Atoms in Molecules", (April 2002). (Host: Prof. Imre G. Csizmadia).

3. Lecture: McMaster Undergraduate Chemical Society Lecture Series, *McMaster University (Hamilton, ON, Canada)*. "Chemistry from the Electron and Pair Densities: Focus on Aromaticity", (Fall, 2001).

2. Seminar: *Dept. of Chemistry, Brock University (St. Cathrines, ON, Canada).* "Criteria of Chemical Bonding from the Topology of the Density", (26 Sept. 2001). (Host: Prof. Heather Gordon).

1. Graduate Seminar: *Dept. of Chemistry, McMaster University (Hamilton, ON, Canada).* "The properties of Morphine, the Oripavine PET, and Enkephalins from Fragments", (3May 2001).

2.2 Conference Presentations
(Presenting Author is underlined)

155 Matta, C. F. "ATP Synthase: More than just a biocatalyst?", *Distinguished Lectures in Quantum Crystallography and Related Fields,* Warsaw University, Warsaw (16 November 2023). *Plenary*

154 Matta, C. F. "ATP Synthase Beyond Catalysis", *8th International Conference Nanobiophysics: Fundamental and Applied Aspects,* NBP-2023, Institute of Physics of the National Academy of Science of Ukraine (NAS), Kiev, Ukraine (3-6 October 2023). *Plenary*

153 Matta, C. F. "1923-2023, The Centenary of the Birth of René Thom", Institut des hautes études scientifiques (IHÉS) [Institute of Advanced Scientific Studies], Paris-Saclay, (France) – (20-23 September 2023). *Plenary*

152 Matta, C. F. "Electron Localization-Delocalization Matrices (LDMs): A New General Purpose Molecular Descriptor and Design Tool", Symposium B9: New Trends in Nanoscience and Nanotechnology: Innovative Synthesis, Novel Properties, Theory and Challenges, 31st International Materials Research Congress 2023, Cancún, (Mexico) – 16 August - (13-18 August 2023). *Oral*

151 Matta, C. F. "The electrostatic potential of ATP Synthase", Symposium C3: Equilibrium and Beyond-Equilibrium Self-Organization in Soft Materials: A Symposium in Honor ID Prof. Juan De Pablo, 31st International Materials Research Congress 2023, Cancún, (Mexico) – 15 August - (13-18 August 2023). *Oral*

150 Matta, C. F. "Electron Localization-Delocalization Matrices (LDMs): A New General Purpose Molecular Descriptor and Design Tool", Symposium A9: Challenges Materials Technologies Energy Conversion, Saving Storage (MATECSS), 31st International Materials Research Congress 2023, Cancún, (Mexico) – 14 August - (13-18 August 2023). *Oral, Invited*

149 Matta, C. F. "Quantum chemistry for high energy materials design"; First IOCD North/South Collaborative Workshop on Energy (Pre-IMRC2023 Symposium / Workshop), Cancún, (Mexico) – 12 August - (11-12 August 2023). *Oral, Invited*

148 Matta, C. F. "Causal mapping: Some observations and questions by a chemist", Quantum Crystallography Session, 17th International Congress on Logic, Methodology and Philosophy of Science and Technology (17th CLMPST) 2023, Buenos Aires, (Argentina) (24-29 July 2023). *Oral, Invited*

147 Massa, L.; Matta, C. F. "The Total Energy from X-Ray Electron Density?", Quantum Crystallography Session, The American Crystallographic Association (ACA) 73rd Annual Meeting, Baltimore, Maryland (USA) (7-11 July 2023). *Oral, Invited*

146 Matta, C. F.; Mortera-Carbonell, A. d. J.; Andreson, J. S. M.; Massa, l. "Extension of Bright Wilson's Justification of the First Hohenberg Kohn Theorem to Non-Nuclear Maxima (NNM)", Quantum Crystallography Session, The American Crystallographic Association (ACA) 73rd Annual Meeting, Baltimore, Maryland (USA) (7-11 July 2023). *Oral, Invited*

145 Matta, C. F., Cook, R.; Ayers, P. W. "Electron Localization-Delocalization Matrices (LDMs): A New Predictor of Molecular Properties", *Canadian Chemistry Conference & Exhibition (CSC 2023)*, Vancouver, BC, Canada, (4 - 8 June 2023). *Oral*

144 Matta, C. F., Vigneau, J.-N.; Fahimi, P.; Nguyen-Dang, T.-T. "ATP Synthase Beyond Catalysis", *Canadian Chemistry Conference & Exhibition (CSC 2023)*, *Oral*

Vancouver, BC, Canada, (4 - 8 June 2023).

143 Massa, L.; Matta, C. F. "The Kernel Energy Method (KEM) Including Electric Field Perturbation", *Canadian Chemistry Conference & Exhibition (CSC 2023)*, Vancouver, BC, Canada, (4 - 8 June 2023). *Oral, invited*

142 Sullivan, A. D.; Smith, E. R.; Smith, F. M.; Fields, T. M.; Harriott, T. A.; Majaess, D.; Massa, L.; Matta, C. F.: "Preliminary investigation of separate potential molecular carriers for two different DIB families", *ChemCon2023 (Atlantic Chemistry Convention)*, Dalhousie University, NS (Canada), (25-27 May 2023). BEST STUDENT PRESENTATION AWARD *Oral*

141 Matta, C. F.: Panel: Construire des ponts dans la communauté de recherche francophone et francophile dans les provinces atlantiques [Trans. Building bridges in the francophone and francophile research community in the Atlantic provinces], *Acfas-Acadie Assemblé génerale annuelle [Annual general assembly of Acfas-Acadie],* (19 May 2023), Halifax, NS, Canada. *Invited Panelist*

140 Matta, C. F.: "Réflexion sur l'apport de la culture française en science [Trans : Reflexions on the contribution of the french culture in science]" ; Colloque : 100 ans de recherche, 100 ans de transformations? [Trans. Colloquium on 100 years of research, 100 years of transformation] *Acfas 90th Congress,* (8 – 12 May 2023), Montreal, QC, Canada. *Invited Oral communication & Invited Panelist*

139 Matta, C. F.: "Théorie des graphes et des réseaux : une théorie transdisciplinaire de grande envergure [Trans : Graph and network theory : A far-reaching theory]" ; Colloque sur la transdisciplinarité et évolution des savoirs : fondements et pratiques [Trans. Colloquium on transdisciplinarity and the evolution of knowledge: fondamentals and practice] *Acfas 90th Congress,* (8 – 12 May 2023), Montreal, QC, Canada. *Invited Lecture*

138 Sullivan, A. D.; Smith, E. R.; Smith, F. M.; Fields, T. M.; Harriott, T. A.; Majaess, D.; Massa, L.; Matta, C. F.: "Insight into diffuse interstellar bands via a functional group analysis tied to RASCALL", *Maritime Astronomy (STARS) Group Meeting*, Mount Allison University, NB (Canada), (April 2023). *Oral presentation*

137 Matta, C. F.; "ATP Synthase: An Enzyme Beyond a mere Biological Catalyst", World Chemistry Forum 2023 (WCF-2023), Budapest, (Hungary) (12-14 April 2023). *Invited Keynote Lecture*

136 Smith, E. R.; Sullivan, A. D.; Smith, F. M.; Fields, T. M.; Harriott, T. A.; Majaess, D.; Massa, L.; Matta, C. F.; "Exploring Diffuse Interstellar Band Dependencies on Near-infrared Reddening", 241st Meeting o the American Astronomical Society (AAS 241), Seattle, Washington (USA) (8 – 12 January 2023). *Poster*

135 Sullivan, A. D.; Smith, E. R.; Smith, F. M.; Fields, T. M.; Harriott, T. A.; Majaess, D.; Massa, L.; Matta, C. F.; "Separate Molecular Carriers for the Mary Lea Heger DIBs at 5780 and 5797 Å", 241st Meeting o the American Astronomical Society (AAS 241), Seattle, Washington (USA) (8 – 12 January 2023). *Poster*

134 Matta, C. F.; "Novel Functions of ATP Synthase Over and Above its Role as a Catalysis", *The 14th General Assembly of the African Academy of Sciences and the 2nd Connecting Minds Africa Meeting 2nd Connecting Minds Africa* *Invited Keynote*

	Conference (CoMA 2022) - (a parallel event of the *World Science Forum* 2022), Cape Town (South Africa) (5-9 Dec. 2022).	*Address*
133	Matta, C. F.; Moderator of "Needs & Technologies for healthy societies with responsive & resilient health systems", (Panelists: Prof. Marleen Temmerman, Prof. Jean-Paul Moatti, Dr. Benjamin Kumwenda, Dr. Nana Ama Amissah, Dr. Dacquin Kasumba, Rapporteur: R. Opisa), *The 14th General Assembly of the African Academy of Sciences and the 2nd Connecting Minds Africa Meeting 2nd Connecting Minds Africa Conference (CoMA 2022)* - (a parallel event of the *World Science Forum* 2022), Cape Town (South Africa) (5-9 Dec. 2022).	*Discussion Panel Moderator*
132	Matta, C. F.; Moderator of "Public Health", (Panelists: Several; Rapporteur: R. Opisa), *The 14th General Assembly of the African Academy of Sciences and the 2nd Connecting Minds Africa Meeting 2nd Connecting Minds Africa Conference (CoMA 2022)* - (a parallel event of the *World Science Forum* 2022), Cape Town (South Africa) (5-9 Dec. 2022).	*Discussion Panel Moderator*
131	Matta, C. F.; Moderator of "Panel Discussion on Research Infrastructure Development in Africa", (Panelists: Prof. Shabaan Khalil, Prof. Malik Maaza, Prof. Fairouz Malek; Rapporteur: R. Opisa), *The 14th General Assembly of the African Academy of Sciences and the 2nd Connecting Minds Africa Meeting 2nd Connecting Minds Africa Conference (CoMA 2022)* - (a parallel event of the *World Science Forum* 2022), Cape Town (South Africa) (5-9 Dec. 2022).	*Discussion Panel Moderator*
130	Matta, C. F.; Moderator of "Panel Discussion on Research Infrastructure Development in Africa", (Panelists: Prof. Shabaan Khalil, Prof. Malik Maaza, Prof. Fairouz Malek; Rapporteur: Gladys Wakaba), *The 14th General Assembly of the African Academy of Sciences and the 2nd Connecting Minds Africa Meeting 2nd Connecting Minds Africa Conference (CoMA 2022)* - (a parallel event of the *World Science Forum* 2022), Cape Town (South Africa) (5-9 Dec. 2022).	*Discussion Panel Moderator*
129	Matta, C. F.; James S. M. Anderson, J. S. M.; Aldo de Jesús Mortera-Carbonell, A. d. J.; Massa, L; "Non-Nuclear Maxima and the Universality of Bright Wilson's Justification of the First Hohenberg-Kohn Theorem", International Conference on Chemical Bonding (ICCB-2022), Lihue- Kauai, Hawaii (USA) (11-16 August 2022).	*Invited Lecture*
128	Matta, C. F.; "The Electrostatic Potential of ATP Synthase and its Biochemical Role Beyond Catalysis", *The 12th Triennial Congress of the World Association of Theoretical and Computational Chemists WATOC 2020,* Vancouver, BC (Canada) (3 - 8 July 2022).	*Invited Lecture*
127	Matta, C. F.; "ATP Synthase: A Moonlighting Enzyme with Unique Functions", *The 12th Congress on Electronic Structure Principles and Applications ESPA2022,* Universidad de Vigo, Vigo (Spain) (21 - 24 June 2022).	*Invited Lecture*
126	Castanedo, L. A. M.; Matta, C. F.; "Prebiotic Thermodynamic "Selection of the Fittest" Anomers", *12th Congress on Electronic Structure Principles and Applications ESPA2022,* Universidad de Vigo, Vigo (Spain) (21 - 24 June 2022).	*Poster*
125	Smith, E. R.; Smith, F. M.; Fields, T. M.; Harriott, T. A.; Majaess, D.; Massa, L.;	*Poster*

Matta, C. F. "On Astrochemistry's Century-old Celestial Mystery", *12th Congress on Electronic Structure Principles and Applications ESPA2022,* Universidad de Vigo, Vigo (Spain) (21 - 24 June 2022).

124	Matta, C. F.; "ATP-Synthase: More than an Enzyme", *II Virtual Meeting of the Nanoscience Division of the Mexican Physics Society, 2021*, Universidad de Guadalajara, Mexico (25 and 28 Oct. 2021).	*Plenary Lecture (Invited)*
123	Matta, C. F.; "Algunas observaciones sobre el mapeo causal (causal mapping) en química" (Some observations on causal mapping in chemistry), *II JFQ 2021: II Jornadas de Fundamentos de Química (Second Workshop on the Foundations of Chemistry)*, Universidad Nacional de la Patagonia San Juan Bosco (UNPSJB) (National University of the Patagonia San Juan Bosco) - Argentina (5 and 7 Oct. 2021).	*Oral (Invited)* *[In Spanish]*
122	Matta, C. F.; Anderson, J.; Massa, L. "Non-Nuclear Maxima and the Universality of Bright Wilson's Justification of the First Hohenberg Kohn Theorem", *Second Discussion Meeting on Quantum Crystallography: Expectations and Reality*, Centre Européen de Calcul Atomique et Moléculaire (CECAM), online meeting (9-12 Sept. 2021).	*Oral (Invited)*
121	Fahimi, P.; Vigneau, J.-N.; Ebert, M.; Cheng, Y.; Matta, C. F. "The Electric Field of ATP-Synthase", *Second Discussion Meeting on Quantum Crystallography: Expectations and Reality*, Centre Européen de Calcul Atomique et Moléculaire (CECAM), online meeting (9-12 Sept. 2021).	*Poster (Invited)*
120	Matta, C. F., "The Electric field of ATP Synthase" at the MS-89 Symposium: Quantum crystallography in materials science, in: *Congress and General Assembly of the International Union of Crystallography **IUCr-2021***, Prague, Czech Republic, (14-22 August 2021).	*Oral (invited)*
119	Matta, C. F.; Anderson, J. S. M.; Massa, L. "Non-Nuclear Maxima and the Universality of Bright Wilson's Justification of the First Hohenberg Kohn Theorem"; *24th Conference of the International Society for the Philosophy of Chemistry (ISPC 2021)*, Buenos Aires, Argentina (July 12 - 23, 2021).	*Oral (invited)*
118	Castanedo, L. A. M.; Matta, C. F. "Ácidos nucleicos primordiales" (Primordial Nucleic Acids)); *QCT-MEX Simposio Virtual 2020 (The 2020 Virtual Symposium onf Quantum Chemical Topology (QCT) - Mexico),* México City, Mexico, (December 14 - 15, 2020).	*Oral (invited)* *[In Spanish]*
117	Polkosnik, W.; Huang, L; Matta, C. F.; Massa, L. "Quantum Crystallography: N-Representability Big & Small"; *Quantum Crystallography Online Meeting 2020 QCrOM2020 (International Union of Crystallography – Commission on Quantum Crystallography),* Paris, France, (August 26 - 29, 2020).	*Oral (invited)*
116	Matta, C. F. "Title TBA"; *12th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2021), Vancouver, Canada* (Originally scheduled for August 16 - 21, 2020, delayed to 2021 due to COVID19 Pandemic).	*Oral*
115	Matta, C. F. "Title TBA"; *7th International Conference on Chemical Bonding,*	*Oral (invited)*

ICCB, Kauai, Hawaii, USA (Originally scheduled for Aug. 9-13, 2020, delayed to 2021 due to COVID19 Pandemic).

114	Matta, C. F. "Title TBA"; *BioVisionAlexandria (BVA) 2020, The World Biological Forum's Annual Conference, Bibliotheca Alexandrina, Alexandria, Egypt* (Originally scheduled for Apr. 9-11, 2020, delayed due to COVID19 Pandemic).	*Oral (invited)*
113	Matta, C. F. "Electron Localization-Delocalization Matrices (LDMs)", *2020 CERMM Annual Symposium,* Centre for Research in Molecular Modeling of Concordia University (CERMM), Montreal, Canada (7 February 2020).	*Oral (Invited)*
112	Nasr, M. A.; Dovbeshko, G. I.; Bearne, S. L.; El-Badri, N.; Matta, C. F. "Heat Shock Proteins in the "Hot" Mitochondrion: Identity and Putative Roles", *6th International Conference: Nanobiophysics: fundamental and applied aspects,* NBP-2019, Institute of Physics of the National Academy of Science of Ukraine (NAS), Kiev, Ukraine (1-4 October 2019).	*Oral*
111	Matta, C. F. "Controlled Thermogenesis in the Mitochondrion", *6th International Conference: Nanobiophysics: fundamental and applied aspects,* NBP-2019, Institute of Physics of the National Academy of Science of Ukraine (NAS), Kiev, Ukraine (1-4 October 2019).	*Oral (Plenary)*
110	Castanedo, L. A. M.; Matta, C. F. "Does the thermodynamic stability of canonical nucleosides-nucleotides a possible driver in early evolution?", *Congress of Theoretical Chemists of the Latin Expression Quitel/Chitel XLV*, Montreal, Canada (25-30 Aug. 2019).	*Oral*
109	Castanedo, L. A. M.; Lamar, A. S.; Boado, C. M.; Nuez-Veulens, A. d. l.; Matta, C. F. "Genoprotection by Complexation: The Case of Phyllanthus orbicularis K Extract", *Congress of Theoretical Chemists of the Latin Expression Quitel/Chitel XLV*, Montreal, Canada (25-30 Aug. 2019).	*Poster*
108	Fahimi, P.; Castanedo, L. A. M.; Nguyen-Dang, T.-T.; Matta, C. F. "Electrical feedback regulation of the mitochondrial inner membrane electrical potential", *Congress of Theoretical Chemists of the Latin Expression Quitel/Chitel XLV*, Montreal, Canada (25-30 Aug. 2019).	*Poster*
107	Cheng, Y.; Matta, C. F. "A Possible Fundamental Role of the Intrinsic Electric Field of ATP Synthase", *102nd Canadian Chemistry Conference & Exhibition (CSC 2019)*, Québec City, QC, Canada, (3 - 7 June 2019).	*Oral*
106	Matta, C. F., Massa, L. "Teoría de la información: ¿Un nivel irreducible independiente de descripción de los sistemas biológicos complejos?" [Information Theory: A Irreducible Independent Level of Description of Complex Biological Systems?], *1º Jornadas de Historia, Filosofía y Didáctica de la Química del Cono Sur* (First Meeting on the History, Philosophy and Didactics of Chemistry of the Southern Cone), Buenos Aires, Argentina (13-15 May 2019).	*Oral, Plenary (Invited) [In Spanish]*
105	Matta, C. F.; Massa, L. "Kidneys, Mitochondria, and Maxwell's Demon: An Information Theoretic Investigation"; *World Chemistry - Quantum Physics -*	*Oral (Keynote Address)*

Congress 2018 (WCC 2018), Stockholm, Sweden (10-13 December 2018).

104 Monteserín Castanedo, L. A.; Matta, C. F. "On the thermodynamic stability and the natural selection of canonical nucleosides in the prebiotic evolution of life", *International Union of Crystallography (IUCr)'s Sagamore XIX Conference on Quantum Crystallography (QCr) (Sagamore - 2018)*, Halifax, NS, Canada (8-13 July 2018). *Poster* (POSTER PRIZE)

103 Monteserín Castanedo, L. A.; Lamar, A. S.; Boado, C. M.; Nuez-Veulens, A. d.l.; Fernández, R. R.; Matta, C. F. "A "direct" mechanism for the action of the genoprotectors extracted from the Cuban plant Phyllanthus Orbicularis K", *International Union of Crystallography (IUCr)'s Sagamore XIX Conference on Quantum Crystallography (QCr) (Sagamore - 2018)*, Halifax, NS, Canada (8-13 July 2018). *Poster*

102 Cheng, Y.; Keith, T. A.; Massa, L.; Matta, C. F. "Interpretation of the Kernel Energy Method (KEM) using the Theory of Interacting Quantum Atoms (IQA)", *International Union of Crystallography (IUCr)'s Sagamore XIX Conference on Quantum Crystallography (QCr) (Sagamore - 2018)*, Halifax, NS, Canada (8-13 July 2018). *Poster*

101 Sowlati-Hashjin, S.; Matta, C. F. "Atomic and Molecular Properties of Diatomic Molecules in External Electric Fields", *International Union of Crystallography (IUCr)'s Sagamore XIX Conference on Quantum Crystallography (QCr) (Sagamore - 2018)*, Halifax, NS, Canada (8-13 July 2018). *Oral (invited)*

100 Matta, C. F.; Cook, R.; Sumar, I.; Ayers, P. W. "Localization-Delocalization Matrices", *24th Congress and General Assembly of the International Union of Crystallography (IUCr - 2017)*, Hyderabad, India (21-28 August 2017). *Oral (invited)*

99 Matta, C. F. "Molecules as Networks", *CECAM Discussion Meeting - Quantum Crystallography: Current Developments and Future Perspectives*, Centre Européen de Calcul Atomique et Moléculaire, Nancy, France (19-20 June 2017). *Oral (invited)*

98 Cook, R.L.; Matta, C. F. "Localization-delocalization Matrices (LDM): A Source for Electron Density Based Descriptors for Use in Physical and Biological Modeling", *100th Canadian Chemistry Conference & Exhibition (CSC 2017)*, Toronto, ON, Canada, (28 May - 1 June 2017). *Oral (invited)*

97 Massa, L.; Timm, M.; Huang, L., Matta, C. F. "Electron Localization/ Delocalization Matrices (LDMs) and the Electron-density-weighted Connectivity Matrices of a Large Molecule from Fragments: The Challenging Case of a Finite Graphene Nanoribbon", *100th Canadian Chemistry Conference & Exhibition (CSC 2017)*, Toronto, ON, Canada, (28 May - 1 June 2017). *Oral (invited)*

96 Monteserín-Castanedo, L. A.; Matta, C. F. "Does the Thermodynamic Stability of Canonical Nucleosides over Non-Canonical Nucleosides a Possible Driver in Early Evolution?", *100th Canadian Chemistry Conference & Exhibition (CSC 2017)*, Toronto, ON, Canada, (28 May - 1 June 2017). *Poster*

95 Monteserín-Castanedo, L. A.; Lamar, A. S.; Matta, C. F. "A Computational Study of Genoprotection by Natural Products found in Phyllanthus Orbicularis *Poster*

K Extract", *100th Canadian Chemistry Conference & Exhibition (CSC 2017)*, Toronto, ON, Canada, (28 May - 1 June 2017).

94 Arabi, A. A.; Matta, C. F. "Investigation of the Molecular Electrostatic Potentials and the Average Electron Densities of Non-Classical Bioisosteres", *253rd American Chemical Society (ACS) National Meeting & Exposition, Advanced Materials, Technologies, Systems & Processes*, San Francisco, California, USA, (2-6 April 2017). *Oral*

93 Matta, C. F. "What Happens to Chemical Bond when the Identity of an Atom Changes due to a Nuclear Transmutation? A Case Study", *ChemBond 2016: Chemical Bonding in Position Space*, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, (27 Nov. - 1 Dec., 2016). *Oral (invited)*

92 Massa, L.; Polkosnik, W.; Matta, C. F.; Huang, L. "A New Understanding in Context of X-Ray Quantum Crystallography (QCr) and the Kernel Energy Method (KEM)", *Crystallography 2016: International Conference on Applied Crystallography (ConferenceSeries.com – 748th Conference),* Houston, Texas, USA, (17-19 October 2016). [Abstract published in the *Journal of Material Science and Engineering* **Volume 5**, Issue 8 (Suppl), p. 64 (2016)]. *Oral*

91 Massa, L.; Polkosnik, W.; Matta, C. F.; Huang, L. "A Revolutionary Idea in Context of X-ray Quantum Crystallography (QCr) and the Kernel Energy Method (KEM)", *44th Middle Atlantic Regional Meeting (MARM 2016) of the American Chemical Society*, Riverdale, New York, USA, (9-12 June, 2016). *Oral*

90 Matta, C. F.; Terrabuio, L. A.; Haiduke, R. L. A. "Diuorodiazirine (CF_2N_2): A Quantum Mechanical Study of the Electron Density in the Ground- and Excited-Electronic States", *99th Canadian Chemistry Conference & Exhibition (CSC 2016)*, Halifax, NS, Canada, (5-9 June, 2016). *Oral*

89 Matta, C. F.; Sumar, I.; Cook, R.; Ayers, P. W. "Electron Localization-Delocalization Matrices (LDM): Definition and Applications", *99th Canadian Chemistry Conference & Exhibition (CSC 2016)*, Halifax, NS, Canada, (5-9 June, 2016). *Oral*

88 Arabi, A. A.; Matta, C. F. "Average Electron Densities and Electrostatic Potentials of the Nonclassical Bioisosteric Groups in Acetic Acid and Methylsquarate", *99th Canadian Chemistry Conference & Exhibition (CSC 2016)*, Halifax, NS, Canada, (5-9 June, 2016). *Oral*

87 Matta, C. F. "Graph Theoretical Molecular Fingerprinting starting from Electron Density Distributions", *2016 Canadian Chemical Crystallography Workshop (Canadian National Committee for Crystallography)* – Saint Mary's University, Halifax, NS, Canada, (May 30th - June 3rd) *Oral (invited)*

86 Terrabuio, L. A.; Haiduke, R. L. A.; Matta, C. F. "Diuorodiazirine (CF_2N_2) in the Ground- and Excited-Electronic States: A Study of the Electron Density", *L'INRS - 2016 Symposium on Molecules and Laser Fields (Andre D. Bandrauk Honorary Symposium),* Orford, Québec, Canada, *(4-7 may 2016)*. *Oral (invited)*

85 Terrabuio, L. A.; Haiduke, R. L. A.; Matta, C. F. "Difluorodiazirine (CF_2N_2): A Comparative Quantum Mechanical Study of the First Triplet and First Singlet *Poster*

Excited States", *L'INRS - 2016 Symposium on Molecules and Laser Fields (Andre D. Bandrauk Honorary Symposium),* Orford, Québec, Canada, *(4-7 may 2016)*. *(invited)*

84 Sumar, I.; Cook, R.; Ayers, P. W.; Matta, C. F. "From Chemical Graph Theory to the Electronic Structure Fingerprinting of Localization-Delocalization Matrices (LDMs) and of Electron Density-Weighted Adjacency Matrices (EDWAMs), *The International Chemical Congress of Pacific Basin Societies (PACIFICHEM) 2015,* Honolulu, Hawaii, USA, *(15-20 Dec. 2015)*. *Oral (invited)*

83 Matta, C. F. "Anneaux-en-molécules: Aromaticité comme distance de similarité à la matrice de localisation et délocalisation (LDM) du benzène" (Rings-in-Molecules: Aromaticity as similarity distance to the localization-delocalization matrix of benzene), *Chitel 2015 (Quitel XLI (41)): Congress of Theoretical Chemists of Latin Expression*; Turin, Italy *(26-31 July 2015)*. *Oral*

[in French]

82 Sumar, I.; Cook, R.; Ayers, P. W.; Matta, C. F. "Las matrices de localización-deslocalización (LDM): Un puente conceptual entre la teoría química de los grafos y la teoría cuántica de los átomos en moléculas" (Localization-delocalization matrices: A bridge between chemical graph theory and the quantum theory of atoms in molecules), *Chitel 2015 (Quitel XLI (41)): Congress of Theoretical Chemists of Latin Expression*; Turin, Italy *(26-31 July 2015)*. *Poster*

[in Spanish]

81 Matta, C. F. "Electron localization-delocalization matrices (LDMs): Recent developments", *Sagamore XVIII Conference on Charge, Spin and Momentum Densities (CSMD), International Union of Crystallography (IUCr), IUCr Commission on Charge, Spin and Momentum Densities*; Santa Margherita di Pula, Sardinia, Italy *(7-12 June 2015)*. *Oral (invited)*

80 Sumar, I.; Cook, R.; Ayers, P. W.; Matta, C. F. "Rings-in-Molecules: Aromaticity as a Similarity Distance to the Localization-Delocalization Matrix (LDM) of Benzene", *Sagamore XVIII Conference on Charge, Spin and Momentum Densities (CSMD), International Union of Crystallography (IUCr), IUCr Commission on Charge, Spin and Momentum Densities*; Santa Margherita di Pula, Sardinia, Italy *(7-12 June 2015)*. (*North American Travel Grant IUCr Award* for graduate student Ismat Sumar to present his work at the conference). *Poster (Award)*

79 Matta, C. F. "The molecular electron density: From topography and topology to abstract art" *3rd International Interdisciplinary Symposium, CroArtScia2015 – Technological Innovations: Art & Science* (27–30 May 2015), Zagreb, Croatia. *Oral (invited)*

78 Matta, C. F. "The definition of electron localization-delocalization matrices (LDMs) & their use as electronic fingerprinting tool in QSAR & molecular similarity", *10th Congress of the World Association of Theoretical and Computational Chemists* (WATOC 2014); Santiago, Chile (5-10 Oct. 2014). *Oral (invited)*

77 Timm, M.; Matta, C. F. "The Evolution of Chemical Bonding over the Nuclear Transmutation Reaction Path", *Third Changsha International Workshop on Theoretical and Computational Chemistry with Materials*; Hunan Normal University, Changsha, China (8-10 June 2014). *Oral (invited)*

76 Timm, M. J.; Matta, C. F. "Primary Retention following Nuclear Recoil in β-Decay: Proposed Synthesis of a Metastable Rare Gas Oxide ($^{38}ArO_4$) from ($^{38}ClO_4^-$) and the Evolution of Chemical Bonding over the Nuclear Transmutation Reaction Path", *39th Annual Science Atlantic / CIC Student Chemistry Conference ChemCon2014, Science Atlantic, Acadia University* (22-24 May 2014). **[Science Atlantic Communication Award for best student presentation].** — *Oral*

75 Sumar, I.; Ayers, P. W.; Matta, C. F. "Definition and some Uses of Localization/Delocalization Matrices (LDMs)", *Congress and General Assembly of the International Union of Crystallography (IUCr-2014)*, Montreal, Canada (5-12 Aug. 2014). — *Poster*

74 Sumar, I.; Ayers, P. W.; Matta, C. F. "Definition and some Uses of Localization/Delocalization Matrices (LDMs)", *Third Changsha International Workshop on Theoretical and Computational Chemistry with Materials*, Hunan Normal University, Changsha, China (8-10 June 2014). — *Poster (invited)*

73 Matta, C. F.; Huang, L.; Massa, L. "A Graphene Flake Under External Electric Fields Reconstructed From Field-Perturbed Kernels", *Third Changsha International Workshop on Theoretical and Computational Chemistry with Materials*, Hunan Normal University, Changsha, China (8-10 June 2014). — *Poster (invited)*

72 Matta, C. F. "Some Effects of Electric Fields on Bonding and Reactivity", *Symposium: Advances in Quantum Chemical Topology, Mexico City, Mexico* (7-10 Oct., 2013). — *Oral (invited)*

71 Matta, C. F. "Computational Investigations of Field Effects on Chemical Bonding and Reactivity", *Gordon Research Conference (GRC) on Electron Distribution and Chemical Bonding: Pushing the Limits of Experimental and Theoretical Charge and Spin Density Studies, Les Diablerets, Switzerland* (2-7 June, 2013). — *Oral (invited)*

70 Matta, C. F., Sowlati-Hashjin, S. "Properties of the Chemical Bond under External Electric Fields in Homonuclear and Heteronuclear Diatomics", *96th Canadian Chemistry Conference & Exhibition (CSC 2013)*, Québec, QC, Canada, (26-30 May, 2013). — *Oral (invited)*

69 Sowlati-Hashjin, S.; Matta C. F.; Bandrauk, A. D. "Dipole Moment Surface of the $CH_4 + X \rightarrow CH_3 + HX$ (X = F, Cl) Reactions from Atomic Dipole Moment Surfaces, and the Origin of the Sharp Peak in the Dipole Moment near the Transition State", *96th Canadian Chemistry Conference & Exhibition (CSC 2013)*, Québec, QC, Canada, (26-30 May, 2013). — *Oral (invited)*

68 L. Massa; Matta, C. F.; Keith, T. A. "Topological Properties of the Electron Density: Examples from Quantum Chemistry and Quantum Crystallography", *96th Canadian Chemistry Conference & Exhibition (CSC 2013)*, Québec, QC, Canada, (26-30 May, 2013). — *Oral (invited)*

67 Matta, C. F.; Sowlati-Hashjin, S. "The Chemical Bond under External Electric Fields: A Quantum Chemical Study of Diatomics", *The 39th International Congress of Theoretical Chemists of Latin Expression, Granada, Spain* (30 June - — *Oral*

[In Spanish]

5 July 2013).

66 Matta, C. F.; Huang, L.; Massa, L. "A graphene flake under external electric fields reconstructed from field-perturbed kernels", *Symposium: Advances in Quantum Chemical Topology, Mexico City, Mexico* (7-10 Oct. 2013). *Poster [In Spanish]*

65 Matta, C. F.; Huang, L.; Massa, L. "A graphene flake under external electric fields reconstructed from field-perturbed kernels", *The 39th International Congress of Theoretical Chemists of Latin Expression, Granada, Spain* (30 June - 5 July 2013). *Poster [In Spanish]*

64 Matta, C. F.; "A Tribute to Richard Bader: Introductory Presentation", *Sagamore XVII Conference on Charge, Spin and Momentum Densities (CSMD), International Union of Crystallography (IUCr), IUCr Commission on Charge, Spin and Momentum Densities*; Kitayuzawa, Hokkai-do, Japan *(15-20 July 2012)*. *Oral (invited)*

63 Matta, C. F.; Massa, L.; Keith, T. A. "Richard F. W. Bader (1932-2012): The Pioneer of the Topological Analysis of the Charge Density and of the Quantum Theory of Atoms in molecules (QTAIM)", *Sagamore XVII Conference on Charge, Spin and Momentum Densities (CSMD), International Union of Crystallography (IUCr), IUCr Commission on Charge, Spin and Momentum Densities*; Kitayuzawa, Hokkai-do, Japan *(15-20 July 2012)*. *Poster*

62 Huang, L.; Matta, C. F.; Massa, L. "Anionic Hydrogen Clusters (H_{2n+1}^-) as a Chemical Source of Diffuse Interstellar Bands and Possible Candidates for Hydrogen Storage", *Sagamore XVII Conference on Charge, Spin and Momentum Densities (CSMD), International Union of Crystallography (IUCr), IUCr Commission on Charge, Spin and Momentum Densities*; Kitayuzawa, Hokkai-do, Japan *(15-20 July 2012)*. *Poster*

61 Matta, C. F.; Arabi, A. A.; Sowlati-Hashjin, S.; Bandrauk, A. D. "The Effect of Strong External Electric Fields on Reactions Involving Proton and Hydrogen Atom Transfer", *Sagamore XVII Conference on Charge, Spin and Momentum Densities (CSMD), International Union of Crystallography (IUCr), IUCr Commission on Charge, Spin and Momentum Densities*; Kitayuzawa, Hokkai-do, Japan *(15-20 July 2012)*. *Poster*

60 Matta, C. F.; Bendeif, E.-E.; Stradiotto, M.; Fertey, P.; Lecomte, C. "Can a Formally Zwitterionic Rhodium(I) Complex Emulate the Charge Density of a Cationic Rhodium(I) Complex? A Combined Synchrotron X-Ray and Theoretical Charge Density Study", *Sagamore XVII Conference on Charge, Spin and Momentum Densities (CSMD), International Union of Crystallography (IUCr), IUCr Commission on Charge, Spin and Momentum Densities*; Kitayuzawa, Hokkai-do, Japan *(15-20 July 2012)*. *Poster*

59 Matta, C. F.; Wallace, S.; Huang, L.; Massa, L.; Bernal, I. "New Structures of Hydronium Cation Clusters", *Sagamore XVII Conference on Charge, Spin and Momentum Densities (CSMD), International Union of Crystallography (IUCr), IUCr Commission on Charge, Spin and Momentum Densities*; Kitayuzawa, Hokkai-do, Japan *(15-20 July 2012)*. *Poster*

58 Matta, C. F.; Arabi, A. A.; Sowlati-Hashjin, S.; Bandrauk, A. D. "The Effect of Strong External Electric Fields on Reactions Involving Proton and Hydrogen Atom Transfer", *First Changsha International Workshop on Theoretical and Computational Chemistry with Materials*; Hunan Normal University, Changsha, China (8, 9 June 2012). *Oral (invited)*

57 Matta,C. F.; Arabi, A. A.; Sowlati-Hashjin, Bandrauk, A. D. "L'effet des champs externes sur les chemins de réaction impliquant le transfert d'hydrogène ou de proton", *80e Congrès de l'Association francophone pour le savoir (ACFAS)*, Colloque : Simulations numériques en chimie et biochimie, Montréal, QC, Canada (7-11 May 2012). *Oral (invited)* *[in French]*

56 Sowlati-Hashjin, S.; Matta, C. F.; Bandrauk, A. D. "Atomic Origins of the Dipole and Polarizability Enhancement Near the Transition States of X + H-CH_3 --> XH + CH_3 (X=F, Cl)", *95th Canadian Chemistry Conference & Exhibition (CSC 2012), Calgary, Canada* (26–30 May 2012). *Poster*

55 Sowlati-Hashjin, S.; Matta, C. F. "Are Extended Structures Based on C52–Viable?", *95th Canadian Chemistry Conference (CSC 2012), Calgary, Canada* (26–30 May 2012). *Poster*

54 Matta, C. F.; Wallace, S.; Huang, L.; Massa, L.; Bernal, I. "New Structures of Hydronium Cation Clusters", *First Changsha International Workshop on Theoretical and Computational Chemistry with Materials*, Hunan Normal University, Changsha, China (8, 9 June 2012). *Poster*

53 Matta, C. F.; Bendeif, E.-E.; Stradiotto, M.; Fertey, P.; Lecomte, C. "Can a Formally Zwitterionic Rhodium(I) Complex Emulate the Charge Density of a Cationic Rhodium(I) Complex? A Combined Synchrotron X-Ray and Theoretical Charge Density Study", *First Changsha International Workshop on Theoretical and Computational Chemistry with Materials*, Hunan Normal University, Changsha, China (8, 9 June 2012). *Poster*

52 Huang, L.; Matta, C. F.; Massa, L. "Anionic Hydrogen Clusters (H_{2n+1}^-) as a Chemical Source of Diffuse Interstellar Bands and Possible Candidates for Hydrogen Storage", *First Changsha International Workshop on Theoretical and Computational Chemistry with Materials*, Hunan Normal University, Changsha, China (8, 9 June 2012). *Poster*

51 Matta, C. F.; Arabi, A. A.; Sowlati-Hashjin, S.; Bandrauk, A. D. "The Effect of Strong External Electric Fields on Reactions Involving Proton and Hydrogen Atom Transfer", *First Changsha International Workshop on Theoretical and Computational Chemistry with Materials*, Hunan Normal University, Changsha, China (8, 9 June 2012). *Poster*

50 Matta, C. F.; Massa, L.; Keith T. A. "Richard F. W. Bader (1932-2012): The Pioneer of the Topological Analysis of the Charge Density and of the Quantum Theory of Atoms in molecules (QTAIM)", *First Changsha International Workshop on Theoretical and Computational Chemistry with Materials*, Hunan Normal University, Changsha, China (8, 9 June 2012). *Poster*

49 Matta, C. F. "An Introduction to the Quantum Theory of Atoms in Molecules. Part I: The Foundations", *2011 International School on Charge Density – Theory and Practice, International Union of Crystallography & Zaragoza University, Jaca, Huesca, Spain* (Aug. 30 – Sept. 4, 2011). *Oral (invited)*

48 Matta, C. F. "An Introduction to the Quantum Theory of Atoms in Molecules. Part II: Applications", *2011 International School on Charge Density – Theory and Practice, International Union of Crystallography & Zaragoza University, Jaca, Huesca, Spain* (Aug. 30 – Sept. 4, 2011). *Oral (invited)*

47 Matta, C. F. "A Practical Tutorial on the Quantum Theory of Atoms in Molecules", *2011 International School on Charge Density – Theory and Practice, International Union of Crystallography & Zaragoza University, Jaca, Huesca, Spain* (Aug. 30 – Sept. 4, 2011). *Oral (invited)*

46 Arabi, A. A., Matta, C. F. "Effects of Electric Fields on the Double Proton transfer in Formic Acid Dimer", *11th Annual CERMM (Centre for Research in Molecular Modeling) Symposium*, Concordia University, Montréal, Canada (4-5 June 2011). *Oral*

45 Arabi, A. A., Matta, C. F. "Effects of Electric Fields on the Double Proton transfer in Formic Acid Dimer", *94th Canadian Chemistry Conference & Exhibition (CSC 2011)*, Montréal, Canada, (5-9 June 2011). *Oral*

44 Arabi, A. A., Matta, C. F. "Effects of Electric Fields on the Double Proton transfer in Formic Acid Dimer", *36th Annual APICS-CIC (Atlantic Provinces Council on the Sciences - Chemical Institute of Canada) Chemistry Conference (ChemCon 2011)*, University of Prince Edward Island, PEI, Canada (20-22 May 2011). *Oral*

43 Matta C. F. "Hydrogen-Hydrogen Bonding: A Stabilizing Interaction in Molecules and Crystals", *Central European School on Physical Organic Chemistry: Intermolecular Interactions and Molecular Recognition, Wroclaw, Poland* (8-12 June 2010). *Oral (invited)*

42 Matta, C. F. Conference keynote speaker: "From the Electron Density to Biological Activity: Recent Examples", *Atlantic Computational Life Sciences Challenges Workshop, organized by the National Research Council of Canada (NRC) - Mount Allison University, Sackville, NB, Canada* (14 Nov. 2009). *Oral (invited)*

41 Arabi, A. A., Matta, C. F. "Effect of External Electric Fields on Proton Transfer in the Formic Acid Dimer", *10th Atlantic Theoretical Chemistry Symposium (ATCS)*, University of New Brunswick, Fredericton, NB, Canada (17-19 July 2009). *Oral*

40 Arabi, A. A., Matta, C. F., Weaver, D. F. "Geometrical Similarity of the Disposition of the Electrostatic Potential of Tetrazole and Carboxylic Group at the Root of their Bioisosteric Relationship", *7th Canadian Computational Chemistry Conference (CCCC 7)*, Halifax, Canada (20-24 July 2009). *Poster*

39 Arabi, A. A., Matta, C. F. "Where is Electronic Energy Released from the Gas-Phase Hydrolysis of ATP?", *92nd Canadian Chemistry Conference & Exhibition (CSC 2009)*, Hamilton, Canada (30 May – 3 June 2009). (**2nd Graduate Student** *Poster*

Poster Prize of the CIC Physical Chemistry Division).

38 Arabi, A. A., Matta, C. F. "Where is Electronic Energy Released from the Gas-Phase Hydrolysis of ATP?", *34th Annual Atlantic Provinces Council on the Sciences - Chemical Institute of Canada APICS/CIC Undergraduate Chemistry Conference*, Saint Francis Xavier University, Antigonish, Canada (14-16 May 2009). *Poster*

37 Matta, C. F. "Electron-Density Derived Descriptors in QSAR", *Latest Advances in Drug Discovery Design & Planning Methods, eCheminfo Workshop, Oxford, UK* (21-25 July 2008). *Oral (invited)*

36 Matta, C. F., Boyd, R. J. "A QTAIM Study of DNA Bases", *The VIII Girona Seminar on Aromaticity: Basics and Applications, The University of Girona, Catalonia, Spain* (7 - 10 July 2008). *Oral (invited)*

35 Massa, L.; Matta, C. F. "The Transition State for Formation of the Peptide Bond in the Ribosome", *The 5th European Charge Density Meeting, Gravedona, Italy* (6-11 June 2008). *Oral and Poster (invited)*

34 Matta, C. F., "The Energies of Atoms in Molecules and their Changes in Response to Bond Dissociation and Conformational Change", *Workshop on X-ray Spectroscopies, Lausanne, Switzerland* (30 Jan. – 2 Feb. 2008). *Oral (invited)*

33 Matta C. F., "Some Aspects of Aromaticity within the Framework of Theory of Atoms in Molecules", *Special Seminar to Celebrate the 70th Birthday of Professor Tadeusz Marek Krygowski, Dept. of Chemistry, University of Warsaw, Poland* (9 Feb. 2008). *Oral (invited)*

32 Matta, C. F., Massa, L. "An Electron Density Study of the Mechanism of Peptide Bond Formation in the Ribosome", *The American Chemical Society (ACS) 236th National Meeting and Exposition, Philadelphia, USA* (17-21 Aug. 2008). *Oral*

31 Arabi, A. A., Matta, C. F. "Atomic Partitioning of the Energy of Reaction: The Hydrolysis of a Fuel Biological Molecule, Adenosine 5'-Triphosphate (ATP)", *8th Atlantic Theoretical Chemistry Symposium (ATCS), Cape Breton University, Sydney, NS, Canada* (13-15 Aug. 2008). *Oral*

30 Arabi, A. A., Matta, C. F., "Atomic Partitioning of the Bond Dissociation Energy of First to Third Row Molecules", *Research Day, Mount Saint Vincent University*, Halifax, Canada (Aug. 2008). *Oral*

29 Matta, C. F., Arabi, A. A.; "Atomic Partitioning of the Energy of Reaction: The Hydrolysis of Adenosine 5'-Triphosphate (ATP)", *The 5th European Charge Density Meeting (ECDM5) in Conjunction with DFG 1178 Annual Meeting, Gravedona, Italy* (6-11 June 2008). *Poster*

28 Massa, L.; Matta, C. F. "The Transition State for Formation of the Peptide Bond in the Ribosome", *The 5th European Charge Density Meeting (ECDM5) in Conjunction with DFG 1178 Annual Meeting, Gravedona, Italy* (6-11 June 2008). *Poster and Oral*

27 Matta, C. F. "Bond dissociation in biological molecules: Insight from the *Oral (invited)*

Theory of Atoms in Molecules", *Gordon Research Conference (GRC) on Electron Distribution and Chemical Bonding: Dynamics and Densities, Mount Holyoke College, South Hadley, MA, USA* (1-6 July, 2007).

26 Arabi, A. A., Matta, C. F., "The Role of Mg^{2+} in the Dissociation of High Energy Phosphate Bonds", *Research Day, Mount Saint Vincent University*, Halifax, Canada (Aug. 2007). *Oral*

25 Matta, C. F.; Castillo, N.; Boyd, R. J. "An Atomic Basis for Vibrationless Bond Dissociation Enthalpies in Hydrocarbons", *89th Canadian Chemistry Conference & Exhibition (CSC 2006), Halifax, Canada* (27–31 May 2006). *Oral*

24 Zhurova, E.; Matta, C. F.; Wu, N.; Zhurov, V.; Pinkerton, A. "Experimental and Theoretical Charge Density Study of Estrone". *The 2006 Annual Meeting of the American Crystallographic Association (ACA 2006), Honolulu, USA* (22-27 July 2006). *Poster*

23 Feng, X.; Matta, C. F.; Ban, F.; Stuart Grossert, J.; Weaver, D. F. "Electron spray Ionization Mass Spectrometry Studies on Interactions between Lithium and Other Group 1 Cations with Biologically-Active Amines and Neurotransmitters", *54th American Society for Mass Spectrometry (ASMS) Conference on Mass Spectrometry, Seattle, USA* (28 May - 1 June 2006). *Poster*

22 Taylor, A.; Matta, C. F.; Boyd, R. J. "An Atoms-In-Molecules Study of the Solvated Electron", *89th Canadian Chemistry Conference & Exhibition, Halifax, Canada* (27-31 May 2006). *Poster*

21 Castillo, N.; Matta, C. F.; Grabowski, S.; Boyd, R. J. "An Atomic Basis for the Barrier to Rotation Around the Carbon-Carbon Single Bond in1-fluoro-2-[(Z)-2-fluorovinyl]benzene", *89th Canadian Chemistry Conference & Exhibition, Halifax, Canada* (27-31 May 2006). *Poster*

20 Wolstenholme, D.J.; Matta, C.F.; Cameron, T.S.; "Experimental and Theoretical Electron Density Study of a Highly Twisted Polycyclic Aromatic Hydrocarbon: 4-Methyl-[4] Helicene", *23rd European Crystallographic Meeting (ECM-23), Leuven, Belgium* (6-11 Aug. 2006). *Poster*

19 Boyd R. J., Matta C. F., Castillo N. "Characterization of Extended Weak Bonding in DNA: pi-Stacking (Base-Base), Base-Backbone, and Backbone-Backbone Interactions"; *International Conference of Computational Methods in Sciences and Engineering (ICCMSE 2005), Korinthos, Greece* (21-26 Oct. 2005). *Oral (invited)*

18 Boyd R.J., Matta C.F., Pearson J.K. "Computational Studies on Amino Acids and DNA Components", *88th Canadian Chemistry Conference & Exhibition (CSC 2005), Saskatoon, Canada* (28 May – 1 June 2005). *Oral*

17 Bandrauk A.D., E.-W. S. Sedik, Matta C.F. "Laser Control of Reaction Paths in Laser-Induced Chemical and Ion Molecule Reactions", *10th International Conference on Multiphoton Processes, Orford, QC, Canada (*9-14 Oct. 2005). *Poster*

16 Matta, C. F. "Computational chemistry: A powerful and inexpensive tool for basic and applied research in the life sciences"; *BioVision 2004, The World* *Oral (invited)*

Biological Forum's Annual Conference, Alexandria, Egypt (Apr. 3-5, 2004).

15 Matta, C. F.; Boyd, R. J. "Effects of dimerization and ionization on the electron density distributions of DNA bases", *Gordon Research Conference (GRC) on Electron Distribution & Chemical Bonding: The Chemical Bond - Densities & Dynamics, Mount Holyoke College, MA, USA* (4-9 July 2004). *Poster*

14 Bandrauk, A. D.; Sedik, E. W.; Matta C. F.; "Effect of Laser Phase on Reaction Paths in Laser-Induced Chemical Reactions", *15th Canadian Symposium on Theoretical Chemistry, Université de Montréal, Montreal, QC, Canada* (10-14 July 2004). *Poster*

13 Dobrin, S., Harikumar, R. K.; Matta, C.F.; Petsalakis, I. D; Polanyi, J. C.; Theodorakopoulos, G. "Reactions of dibromo-benzenes and dibromo-xylenes at Si(111) followed one molecule at a time"; *Pre-American Physical Society Workshop on Nanoscience and Nanostructured Materials, Institut National de la Recherche Scientifique, Montreal, QC, Canada* (19-20 March 2004). **(Best Poster Award)**. *Poster*

12 Matta, C. F.: Guest panelist of the quarterly *Toronto Area Drug Discovery Discussions (TAD^3) Meeting on "Solubility"*, *Leslie Dan Faculty of Pharmacy, University of Toronto*, *Toronto, ON, Canada* (30 Sept. 2003). (Organizers: Prof. L. Kotra, *Advanced Chemistry Development Inc.* (ACD), & *Affinuim Pharmaceutical Co.*) *Oral (invited)*

11 Matta C. F., Polanyi, J. C. "Effect of adatom-to-adatom separation on the reactivity of 1,4-dihalobenzenes in reactions on Si(111)7x7 surfaces", *5th Canadian Computational Chemistry Conference(CCCC5-2003), Toronto, Canada* (27-30 July 2003). *Poster*

10 Matta, C. F., Bader, R. F. W. "Atomic and group properties of the genetically-encoded amino acids and their correlations to physicochemical and biological properties", *Chemical Biophysics Symposium 2002, University of Toronto, Canada* (12-14 April 2002). *Poster*

9 Matta, C.F. "The Properties of PEO, Enkephalins, and Morphine from Fragments" *222nd American Chemical Society National Meeting*, *Chicago, USA* (27 August 2001). *Oral*

8 Matta, C.F. "Theoretical synthesis of opioids from fragments", *19th Annual Graduate Students' Symposium, University at Buffalo - The State University of New York, NY, USA* (16-17 May 2001). *Oral*

7 Matta, C.F. "The properties of morphine, PET, and enkephalin from fragments", *Graduate Student Day, McMaster University, Hamilton, Canada* (6 March 2001). **(Best Poster Award)**. *Poster*

6 Matta, C.F. "The properties of morphine, PET, and enkephalin from fragments", *Gordon Research Conference (GRC) on Electron Distribution and Chemical Bonding, Mount Holyoke College, MA, USA* (8-13 July 2001). *Poster*

5 Matta C.F., Hernández-Trujillo, J. "Aromaticity in polycyclic arenes as a manifestation of the delocalisation of the Fermi hole", *14th Canadian* *Poster*

Symposium on Theoretical Chemistry, Carleton University, Ottawa, Canada (4-9 Aug. 2001).

4 Hernández-Trujillo, J., Matta, C. F. "Aromaticity of polyarenes as a manifestation of the delocalization of the Fermi hole", *XLIV National Physics Conference of México (XLIV Congreso Nacional de Física), Morelia, Michoacán, México* (Oct. 2001). *Poster*

3 Bader, R.F.W., Matta, C.F. "Dielectric polarization", *41st Sanibel Symposium: Quantum Theory Project, University of Florida, USA* (24 Feb. - 2 Mar. 2001). *Poster*

2 Matta, C.F., Bader, R.F.W. "Theory of the scanning tunneling microscope as the union of two proper open systems", *Surface Canada 2000: The 17th Canadian Conference on Surface Science, London, ON, Canada* (21-24 May 2000). *Poster*

1 P. H. M. Harrison, C. Cow, S. Sun, J. Britten, C. F. Matta "Crystal structures of 3,4,7,8-tetramethylglycoluril and acyl derivatives, models for polyketide biosynthesis", *80th Canadian Chemistry Conference & Exhibition, Windsor, ON, Canada* (1-4 June 1997). *Oral*

2.3 Non-Technical Public Presentations

10. Guest Speaker: On the benefits and procedures of accreditation by the Canadian Society for Chemistry, *Meeting of Canadian Department Leaders of Physics Programmes, Canadian Association of Physicists*, virtual/Ottawa (17 October 2023).

9. Guest (Opening) Speaker: The Canadian Society for Chemistry System of Accreditation, The 2023 *Canadian Council of University Chemistry Chairs (CCUCC) Meeting*, Canadian Chemistry Conference & Exhibition (CSC 2023), Vancouver, BC, Canada, (4 - 8 June 2023).

8. Guest Speaker (as the Chair of the Canada Research Chairs peer review committee): 2021 *Annual Meeting of the Advisory Committee on Equity, Diversity and Inclusion Policy* (Canada Research Chairs), Ottawa, ON, Canada, (7 December 2021). (Host: Marie-Lynne Boudreau, Director, Policy, Performance, Equity and Diversity - Tri-agency Institutional Programs Secretariat]. [Delivered remotely].

7. Public Lecture: Department of Chemistry, Irving K. Barber Faculty of Science, *University of British Columbia (Okanagan)*, Kelowna, BC (Canada), "Crisscrossing the landscape of leadership in a scholarly environment", (1 March 2021). (Host: Professor Lael Parrott). [Delivered remotely].

6. Convocation Speaker presenting Prof. Lou Massa for admission to the Degree of *Doctor of Humane Letters (Honoris Causa)*, *Mount Saint Vincent University*, Halifax, NS, Canada - 3 November 2019.

5. Invited Speaker: *How Do Research Grant Committees Work? Mount Saint Vincent University* (Halifax, Canada), 1 March 2019. (Moderator: Professor KelleyAnne Malinen).

4. Invited Panellist / Speaker: *Sciences as a foundation of the nutrition/dietetics profession, a session for Applied Human Nutrition students, Mount Saint Vincent University* (Halifax, Canada), 16 January 2019. (Moderator: Sandi Berwick, Chair, Nova Scotia Dietitians Continuing Care Action Group).

3. Speaker: *Research Remixed, Mount Saint Vincent University* (Halifax, Canada), 3 October 2017: "Molecules can be excited and exciting!"

2. Speaker of the week: *Alexandria Rotary Club* (Alexandria, Egypt), 15 August 2017: "مقدمة قصيرة لعلم وتكنولوجيا النانو" [In Arabic: "A Short Introduction to Nanoscience and Nanotechnology"].

1. Convocation Speaker (and Nominator) presenting Nobel Laureate Prof. Ada Yonath for admission to the Degree of *Doctor of Humane Letters (Honoris Causa)*, *Mount Saint Vincent University,* Halifax, NS, Canada - 16 May 2014.

FUNDING AND GRANTS[a]

(Total of **$1,331,069** awarded since 2004)

External Grants & Monetary Awards ($1,188,239)

Amount	Date(s)	Type/Description of Award	Granting Organization
$82,348 (= Euros €56,936)	2023-2026	International Visegrad Strategic Grant titled "*Heme-Proteins in Action: Novel insights into its Biology from Experiment and Theory*" (1/5th of the fund for the Canadian party (Matta)).	International Visegrad Fund (Czech Republic, Hungary, Poland, Slovakia)
$180,000	2022-2027	Discovery Grant "*Theoretical Investigations of some Outstanding Problems in Biophysical Chemistry*"	NSERC[(1)] (Canada)
$15,000[b]	2021	Mitacs Accelerate Entrepreneur funding for PhD student (Lázaro A. M. Castanedo). Project: "Phenols-Functionalized Single-Walled Carbon Nanotubes as a New Class of Antioxidants for the Prevention of Degenerative Diseases".	Mitacs and Lab2Market Inc., (Canada)
$76,595	2020	John R. Evans Leaders Fund "Computational Investigations of Molecular Evolutionary Quantum Biochemistry and Mitochondrial Biophysics"	Canada Foundation for Innovation (CFI), (Canada)
$62,785 (= EGP 1,000,000)	2019-2022	Exceptional Bridging Development Opportunity Programme "Lower Mitochondrial Temperature as a Biomarker for Early Cancer Detection" (Joint Application as the "foreign partner" with Professor Nagwa El-Badri of Zewail City of Science and Technology, Egypt). (1/2 of the fund for the Canadian party (Matta)).	Academy of Scientific Research and Technology (Egypt)
$196,000	2015-2022	Discovery Grant "*Quantum Chemical Investigations of the Inner Mitochondrial Membrane Biochemistry*" (initial grant for 5 years + 1 year extension for COVID + 1 year extension for 3-year service on the NSRC-DG Committee (Evaluation Group))	NSERC[(1)] (Canada)
$8,000	2017	Lady Davis Fellowship in Medicine (USD $7,000)	Lady Davis Fellowship Trust (Israel)
$20,000	2018	Nova Scotia Research and Innovation Graduate Scholarship – Master's (NSGS)	Nova Scotia Government

[a] Chérif F. Matta has been the sole Principal Investigator on all listed grants except otherwise stated.

[b] Withdrawn by us after signing the contract as the time commitment turned out more than expected.

Amount	Date(s)	Type/Description of Award	Granting Organization
		to support my MSc student Mr. Lázaro A. Monteserin Castanedo	
$9,700	2017	Joint Application (with my Student Mr. Lázaro A. Monteserin Castanedo): Emerging Leaders in the Americas Program (ELAP) Scholarship – Stipend for Research Assistantship in my group	Canadian Bureau for International Education, Ottawa, Ontario, Canada
$5,040	2016	Joint Application (with my Student Mr. Lázaro A. Monteserin Castanedo): Wood-Whelan Research Fellowships – Stipend for Research Assistantship in my group (US $4,000 = $5,040)	International Union of Biochemistry and Molecular Biology (IUMB)
$150,000	2010-2015	Discovery Grant	NSERC (Canada)
$64,500	2007-2010	Discovery Grant	NSERC (Canada)
$850	2010	Conference Chair's Fund Award to Cover Conference Registration fees	Gordon Research Conference on Electron Density and Chemical Bonding (USA)
$262,421	2008	Leaders Opportunity Fund	Canada Foundation for Innovation (CFI), (Canada)
$15,000	2004	Polanyi Prize for "exceptional" early-career scholarship	Council of Ontario Universities (Canada)
$80,000	2004-2006	I. W. Killam Stipend	The Killam Trusts (Canada)
$3,000	2004	Killam Research Grant	The Killam Trusts (Canada)
$1,105,891		TOTAL	

(1) NSERC = Natural Sciences and Engineering Research Council of Canada.
(2) CFI = Canada Foundation for Innovation

Internal Grants ($84,705)

Amount	Date(s)	Type/Description of Mount Saint Vincent University Award
$2,000	2023	Travel Grant to present a keynote address at the World Chemistry Forum 2023 (WCF-2023) in Budapest (Hungary).
$1,600	2022-2023	Indigenous-Black-International Science (IBIS) funding for one student
$4,844	2022	Standard Research Grant "Mitochondrial Spectroscopy"
$1,500	2022	Aid to Scholarly Publication "Two projector triple products in quantum crystallography"
$4,917	2019	Standard Research Grant "Mitochondrial Biology at 50°C"
$913	2019	Aid to Scholarly Publication
$4,000	2017	President Conference Grant (Sagamore 2018)
$2,000	2018	Travel Grant to Organize and Chair the International Union of Crystallography's Sagamore 2018 Conference
$2,000	2017	Travel Grant (International Union of Crystallography General Assembly & Conference)
$2,000	2016	Travel Grant (ChemBond2016 Conference)

Amount	Date(s)	Type/Description of Mount Saint Vincent University Award
$5,788	2015	Internal Standard Research Grant "Extending the Kernel Energy Method (KEM) From Electronic Energies to Gibbs (Free) Energies"
$2,000	2015	Travel Grant (Sagamore Conference 2015)
$2,000	2014	Travel Grant (IUCr2014)
$2,000	2013	Travel Grant (CSC2013)
$2,000	2012	Travel Grant (Sagamore Conference 2012)
$2,345	2012	Internal Standard Research Grant
$2,926	2011	Internal Standard Research Grant
$6,375	2010	Internal Standard Research Grant
$1,850	2010	Travel Grant (Gordon Research Conference)
$500	2010	Aid to Scholarly Publication
$1,600	2009	Travel Grant (Symposium Organizer, CSC 2009)
$6,660	2008	Internal Standard Research Grant
$1,600	2008	Travel Grant (8th Girona Seminar on Aromaticity)
$500	2008	Aid to Scholarly Publication
$10,500	2007	Internal Standard Research Grant
$1,800	2007	Travel Grant (Gordon Research Conference)
$10,000	2006	Start-up grant
$77,274	**207-2018**	**TOTAL**

Fund Raising ($15,125)

Funds raised to sponsor the International Union of Crystallography Conference's Sagamore 2018 organized and chaired by C. F. Matta in July 2018 (converted to Can $ when applicable):

- International Union of Crystallography $3,000
- Royal Society of Chemistry (in 5 poster prizes in Journal Subscriptions) $2,500
- McMaster University $2,000
- TKGritsmill Software (AIMAll), Inc. (USA) $1,400
- The Family of the late Prof. Richard F. W. Bader $1,000
- Crystals (Open Access journal) $525

TOTAL: **$10,425**

Funds raised to sponsor the Symposium on Biocomputational Chemistry organized by C. F. Matta within the 90th Canadian Chemistry Conference and Exhibition (CSC 2007) in Winnipeg:

- Chemical Computing Group, Inc. $2,000
- Gaussian, Inc. $1,000
- John Wiley & Sons (Canada), Ltd. $1,000
- Mount Saint Vincent University $700

TOTAL: **$4,700**