CURRICULUM VITAE

Professor Lou Massa

Work Address:

Title: Professor of Chemistry and
Physics Department of Chemistry
and Department of Physics Hunter
College & the Graduate School
City University of New York

695 Park Ave
New York, NY 10065
Tel: +1 (212) 772 4016
E-mail: lmassa@hunter.cuny.edu

Education:

- **Postdoctoral Fellow**, *Brookhaven National Laboratory*, 1966-1969.
- **Ph.D.** (Chemical Physics), *Georgetown University*, 1966.
- **M.Sc.** (Chemical Physics), *Clarkson University*, 1962.
- **B.Sc.** (Physics), *Le Moyne College*, 1961.

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Education:

- **Postdoctoral Fellow**, *Brookhaven National Laboratory*, 1966-1969.
- **Ph.D.** (Chemical Physics), *Georgetown University*, 1966.
- **M.Sc.** (Chemical Physics), *Clarkson University*, 1962.
- **B.Sc.** (Physics), *Le Moyne College*, 1961.

Positions Held at Hunter College – City University of New York (CUNY):

Career Progression:

- 1975-present Full Professor.

- 1972-1975 Associate Professor.
- 1969-1972 Assistant Professor.

Main administrative positions held:

- 1970-1973 President of the Hunter College Senate.
- 1980-1981 President of the Hunter College Faculty Union •

1974-1975 Hunter College Ombudsman

Awards:

- *Honorary degree*, Doctor of Humane Letters, Mount St. Vincent University, *Honoris Causa*.
- American Chemical Society, Westchester *Distinguished Scientist Award 2019.*
- Consultant to International Union of Crystallography, permanent study committee of Quantum Crystallography
- Organizing Committee of Quitel 2019: The Annual Conference of Theoretical Chemists of Latin Expression. August 2019, Montreal
- DeGruyter publication, an early monograph on the subject of Quantum Crystallography
- Keynote lecture Quitel 2019: August 2019, Montreal: Mathematical Problems in Quantum Crystallography & their solutions
- Distinguished Visiting Professor at the United States Naval Research Laboratory.
- Hunter College of the City University of New York (CUNY) President's Award for Excellence in Research.

- U.S. Naval Research Laboratory's Berman Award for Outstanding Science Paper.

Selected Grants (totaling *ca.* US $2.5 million):

- The United States Office of Naval Research (ONR).
- The United States Naval Research Laboratory (NRL).
- The United States National Aeronautics & Space Administration (NASA).
- International Business Machines (IBM).
- The United States National Institutes of Health (NIH).
- The United States National Science Foundation (NSF).

Visiting in residence Appointments:

- Harvard University, MA (USA)
- Brookhaven National Laboratory, Upton NY (USA)
- U.S. Naval Research Laboratory, Washington DC (USA)
- Université de Bordeaux, Bordeaux (France)
- University of London, London (UK)
- IBM Watson Research Laboratory, Yorktown heights, NY (USA)
- University of North Carolina, NC (USA)
- University of New Orleans, NO (USA)
- Grumman Aerospace, Bethpage, NY (USA)
- Naval Surface Warfare Center, Carderock, MD (USA)

Editorial Boards:

- Structural Chemistry (Springer)
- Science & Technology Editor of the City University of New York Television (CUNY – TV).
- Guest Associate Editor of the special issue **Quantum Crystallography**, Journal of Computational Chemistry (JCC), issue 18, (July 5th 2018)

Membership in Learned Societies:

- American Crystallographic Association
- American Physical Society
- American Chemical Society

Selected Lectures and Invited Seminars:

- Princeton University, Princeton, NJ (USA)
- Harvard University, Cambridge, MA (USA)
- Northwestern University, Evanston, IL (USA)
- University of North Dakota, Grand Forks, ND (USA)
- New York Medical College, Valhalla, NY (USA)
- Exxon Research Laboratory, Annandale, NJ (USA)
- IBM Watson Research Laboratory, Yorktown Heights, NY (USA)
- Brookhaven National Laboratory, Upton, NY (USA)
- Naval Research Laboratory, Washington, DC (USA)
- Naval Surface Warfare Center, Carderock, MD (USA)
- Grumman Aerospace, Bethpage, NY (USA)
- University of London, Birkbeck College, London (UK)

- Institut Laue-Langevin, Grenoble (France)
- Université de Bordeaux, Bordeaux (France)
- L'Université de Pau et des Pays de l'Adour, Pau (France)
- McGill University, Montreal (Canada)
- Université de Moncton, Moncton (Canada)
- University of New Brunswick, Fredericton (Canada)
- Weisman Institute of Science, Rehovot (Israel)
- University of Melbourne, Melbourne (Australia)
- University of Houston, Huston, TX (USA)
- Texas A&M, College Station, TX (USA)
- University of Tennessee, Knoxville, TN (USA)
- University of North Carolina, Chapel Hill, NC (USA)
- University of New Mexico, Albuquerque, NM (USA)
- CG47 USS Ticonderoga-Tuscaloosa, MS (USA)
- Quantum Chemistry Winter Institute, Sanibel, FA (USA)
- University of New Hampshire, Durham, NH (USA)
- University of Kentucky, Lexington, KY (USA)
- University of Missouri, Columbia, MO (USA)
- Uppsala University, Uppsala (Sweden)
- Queen's University, Ontario (Canada)
- University of Beijing, Beijing (China)
- University of Coimbra, Paço das Escolas (Portugal)
- University of Saskatchewan, Saskatoon (Canada)
- Rutgers University, Newark, NJ (USA)
- Vassar College, Pougkeepsie, NY (USA)
- Edgewood Arsenal-Aberdeen Proving Ground, Aberdeen, MD (USA)
- City University of New York (CUNY) Academy, Graduate Center, New York, NY (USA)
- Hunter College Department of Mathematics, New York, NY (USA)
- Hunter College Department of Chemistry, New York, NY (USA)
- Hunter College Department of Physics, New York, NY (USA)
- Hunter College Department of Biology, New York, NY (USA)
- University of Hawaii, Honolulu, HI (USA)
- Long Island University, Brooklyn, NY (USA)
- John Jay College, New York, NY (USA)
- State University of New York at Purchase, Purchase, NY (USA)
- University of Arkansas, Fayetteville, AR (USA)
- State University of New York at Buffalo, Buffalo, NY (USA)
- Hunan Normal University, Changsha (China)
- IUCr, Hokkaido (Japan)
- University of California, Davis, CA (USA)

Teaching:

Graduate (Ph.D.) Courses Taught in the last 15 Years:

- X-ray Crystallography
- Quantum Chemistry

- Quantum Physics
- Electrodynamics
- Group Theory
- Advanced Quantum Mechanics
- Theory of Potential Scattering
- X-ray Physics
- Computational Chemistry

Undergraduate (B.Sc. level) Courses Taught in the last 15 Years:

- Computational Chemistry
- Computer Models
- Statistical Mechanics
- Quantum Mechanics
- Thermodynamics
- Kinetic Theory of Matter
- Nuclear Chemistry
- Philosophy of Science
- General Chemistry
- Biochemistry
- Health Sciences
- Physical Chemistry
- Foundations of Science

Publications listed separately: 2 Books, TV series, 237 published papers.

Main Points: a brief accounting.

Professor Lou Massa, is known for being a scientist working in the field of **Quantum Crystallography (QCr)**.

He is the 2019 recipient of an Honorary Doctorate in Humane Letters (D.H.L., *honoris causa*) from Mount Saint Vincent University and he has also been the nominator of his close collaborator Professor Ada Yonath (Nobel Laureate 2009) for the very same degree which she received in 2014 from the same university.

He has been a speaker in dozens of conferences and universities. He is a co-author of more than 230 peer reviewed published papers.

1. THE SCIENCE

1.1 Quantum crystallography: merging experiment (X-ray diffraction) and theory (quantum mechanics)

A series of papers demonstrating the possibility of extracting from X-ray diffraction

experiments more than just the atomic position (a crude representation of electron densities, obtained from a refinement assuming the superposition of spherical atoms) [e.g. *PR* 1969, **177**, 7; *PRL* 1972, **29**, 1363; *IJQC* 1973, **7**, 505]. These seminal papers are at the foundations of the theory of constraining the experimentally-derived structure factors to satisfy the requirements of quantum mechanics including, for example, *N*-Representability of the "experimental" electron density.

Why is this important? Because, now, the way is paved to extract – *from X-ray diffraction experiment* – two-electron properties including, for example, **energy components** [e.g. *Can. J. Chem.* 2018, **96**, 599; *CPL* 2019, **734**, 136650], **electron (de)localization measures** [e.g. *JPCA* 2014, **118**, 11304], **electric-field-perturbed molecular properties** [*Carbon*, 2014, **76**, 310], **bonding descriptors** (e.g. the ones used in the framework of the Quantum Theory of Atoms in Molecules (QTAIM) of Bader [e.g. *JPCA* 2014, **118**, 11304; *Struct. Chem.* 2015, **26**, 1433]).

Lou Massa, demonstrated how one can obtain what is essentially an experimentally-constrained "wavefunction" with all it has to offer beyond the electron density [e.g. *PRB* 1981, **24**, 7018; *PRL* 1985, **55**, 622; *Chem. Script.* 1986, **26**, 469; *IJQC* 1994, **49**, 291].

The work by Massa *et al*. remained early on, limited to smaller molecular (or atomic) crystals until the mid-1990's. Until that time, neither experimental technologies nor computational power were capable of handling molecules of great interest to biological and material science, say proteins or nucleic acids – within the framework of quantum crystallography.

A "quantum leap" happened in the mid-nineties during the yearly summer visits of Lou Massa as a "Distinguished Visiting Professor" at the *Laboratory for the Structure of Matter at the US-Naval Research Laboratory, NRL*, (Washington DC). Massa's yearly stay at NRL was on the invitation of Dr. Jerome Karle, the father of the "direct methods solution" of the phase problem of crystallography for which he won the 1985 Nobel Prize in Chemistry (along with his former classmate H. A. Hauptman).

Together, Karle, Massa, and Massa's former PhD student Lulu Huang (a) coined the term "*Quantum Crystallography*" and (b) generalized it to systems of much larger size by inventing a fragmentation quantum chemical technique they call the Kernel Energy Method (KEM). There are at least 30 papers published by the trio Huang, Massa, and Karle on the topic – too numerous to list (possibly half of these papers appeared in Proceedings of the National Academies of Science, *PNAS*), see the LM list of publications.

Karle appears to have judged this advance of sufficient importance that, in 2006, in his updated biography on the Nobel website he mentions by name Lou Massa and

Lulu Huang in remarks on the method they developed together:

J. Karle, Biographical. Nobel Prize Addendum, April 2006:
(https://www.nobelprize.org/prizes/chemistry/1985/karle/biographical/)

Recently, the International Union of Crystallography (IUCr), in its General Assembly in Hyderabad (India), in 2017, created the permanent study committee, the "IUCr Commission of Quantum Crystallography" – the phrase introduced by the authors in their landmark paper: Massa L, Huang L, Karle J "*Quantum crystallography and the use of kernel projector matrices*" *Int. J. Quantum Chem.* 1995, **56**, 371–384.

Dozens of publications and international conferences have been dedicated to Quantum Crystallography including the IUCr Sagamore Conference organized in Halifax in the summer of 2018. At least a dozen schools, workshops, and conferences – and probably hundreds of publications have been dedicated to the topic since that date. Perhaps the rush of new activity may be viewed as experiment, computational resources, and algorithmic developments related to QCr early ideas. It is amazing to see the field of Quantum Crystallography now flourishing at the fore-front of the science of crystallography with dozens across the world racing to claim priority in its development and application.

1.2 OTHER IMPORTANT CONTRIBUTIONS

For brevity, focus here is on three notable areas where the contributions of Massa have, and continue to be, instrumental at advancing science: *Boron Nanotubes*, *Ribosomal Quantum Chemistry*, and the *Elucidation of the Chemical Source of Diffuse Interstellar Bands* (DIBs).

The work of Massa extends to several other areas with equal importance. To mention, in passing, three examples among *several* others we may cite Massa's computational investigations pushing the boundaries of the Quantum Theory of Atoms in Molecules (QTAIM) [see for e.g. *CPL* 2021, **780**, 138940 on the non-nuclear attractors and the first Hohenberg-Kohn theorem or the profound correspondence about the connections of QTAIM and DFT: Matta CF *Struct. Chem.* 2017, 28, 1591 (published as part of a festschrift in honor of Massa)]. Massa has also important contributions with regards to the structure of water clusters (including ionized, solvated, crystallized, etc. [e.g. *PNAS* 2007, **104**, 16798]) and the prediction of a wide range of explosives' IR signatures to detect and protect US troops from improvised explosive devices (IEDs).

1.2.1 Theoretical prediction of boron nanostructures 10 years before their experimental realization

During a sabbatical year at Harvard University, on the invitation of William

Lipscomb (Nobel Laureate, 1976), Massa and Lipscomb published a series of important papers predicting boron nanostructures [*Inorg. Chem.* 1992, **31**, 2297; *ibid.* 1994, **33**, 5617; *ibid.* 1994, **33**, 5155; *ibid.* 1998, **37**, 6546; *ibid.* 1998, **37**, 6544], a decade before their eventual experimental discovery by a collaboration between groups at Yale University and Brookhaven National Laboratory [see: *JPCB* 2004, **108**, 3967]. This is a dream of theoreticians that, instead of a *post-facto* calculation to justify (or "provide insight into") experiment, here Massa and Lipscomb have *guided* the experiment and made us realize that these technologically appealing new nanostructures are within experimental reach. And indeed they were!

1.2.2 The discovery of the transition state for the peptide-bond formation in the cell's protein factory: the ribosome

In a long-time and close collaboration between Prof. Massa's group and a prominent group at the Weizmann Institute of Science, that of Professor Ada Yonath (the Nobel Laureate 2009 for discovering the atomic structure of the ribosome by developing and using cryo-crystallography), Massa's group has contributed crucially toward the elucidation of the mechanism of peptide bond formation at the active site of present day ribosomes [Massa, Yonath, and Karle *et al*.: *PNAS* 2006, **103**, 13327; Massa L, Matta CF, Yonath A, and Karle J. Chapt. 16 in *Quantum Biochemistry*; Matta CF (Ed.) Wiley-VCH, Weinheim (2010)]. This work has been highlighted in a full cover article in *Chemical & Engineering News (C&EN)* [Borman S. "*Protein factory reveals its secrets: Researchers picture and poke the ribosome to learn how it works*" *C&EN* 2007, **85**(*8*), 13-16].

Later, Massa and Yonath extended the work to the evolutionary precursor of present day ribosomes (the proto-ribosome) [see: *PNAS*, 2013, **110**, 14900].

1.2.3 Pioneering computational chemistry of Diffuse Interstellar Bands (DIBs)

In a series of early papers, Massa proposed ionic hydrogen clusters as possible sources of the enigmatic diffuse interstellar bands (DIBs) [e.g. Massa *et al*.: *Nature* 1973, **245**, 31; *Astrophys. J.* 1974, **189**, 605; *Nature*, 1979, **278**, 332; *JCP* 1981, **75**, 5393].

More recently, based on quantum chemical calculations, Massa *et al.* refined the earlier calculations and proposed additional clusters. The enlarged set constitutes a series of stable anionic hydrogen clusters which Massa *et al*. proposed as potential carriers of DIBs [*JPCA* 2011, **115**, 12451; *ibid.* 2011, **115**, 12445]. **And here again: these clusters – that Massa predicted computationally in 1979 - were observed in mass spectrometry experiments 37 years later in 2016** [Renzler M "*Anionic hydrogen cluster ions as a new form of condensed hydrogen*" *Phys. Rev. Lett.* **117**, 273001 (2016), a paper crediting the theoretical predictions by Massa and Sapse in *Nature*, 1979, **278**, 332].

Most recently, Massa along with Canadian collaborators, report the discovery of four new, formerly overlooked, families of DIBs based on statistical analysis of astronomical high-resolution satellite spectral data [see: *Monthy Notices Royal Astron. Soc. (MNRAS)* 2021, **507**, 5236].

2. SCIENCE HISTORY, PHILOSOPHY OF SCIENCE, AND DISSEMINATION OF SCIENTIFIC CULTURE TO THE WIDER EDUCATED PUBLIC

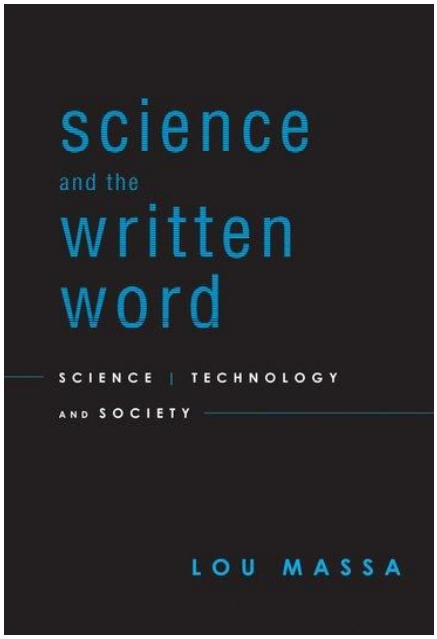
Prof. Massa's contribution in this domain are as follows:

Massa's televised interview programme produced and broadcast by "*City University of New York – TV*" during the 2000-2010 decade and called "*Science and the Written Word*" has featured some of the most influential scientists of our times. These scholars include: **István Hargittai**, **James D. Watson** (Nobel Laureate) as in Watson & Crick, **Dudley R. Herschbach** (Nobel Laureate), **Roald Hoffmann** (Nobel Laureate), **Leon M. Lederman** (Nobel Laureate), **Gertrude B. Elion** (Nobel Laureate), **Rosalyn S. Yalow** (Nobel Laureate) and many others including towering figures such as **Rudolph Pariser**, **Lothar Schäfer**, and **John Archibald Wheeler**. Some of these interviews are available on YouTube (but all have been deposited with the *Chemical Heritage Foundation* and with the *City University of New York TV*):

Science and the Written Word + Lou Massa + CUNY - YouTube**:**

https://www.youtube.com/results?search_query=Science+and+the+Written+Word+%2B+Lou+Massa+%2B+CUNY

In 2011, Massa published his *Oxford University Press* book with the same title based on these interviews.



Massa L. *Science and the Written Word: Science, Technology, and Society*. Oxford University Press, New York, (2011).

This TV-host experience amplified Massa's long experience as a speaker who has given hundreds of presentations at universities and research centers around the world.

Besides his direct contribution to fundamental science, and efforts to popularize scientific culture for the general public, Massa has wide ranging interests including the history, policy, and philosophy of science. As an example of **his advocacy for computational chemistry**, together with Dr. Herb Budd (the former Director of IBM Science Centers (Europe)), the two co-authored a letter to the editor of **Chemistry & Engineering News (C&EN)** entitled "***Using computer simulations to fight Zika***" advocating for resource allocation to combat the Zika virus pandemic by numerical simulations (which would include the use of quantum crystallographic studies in conjunction with structural biology). [See: Budd H, Massa L. *Chem. Eng. News (CE&N)* 2016, **94**, 4].

Highly regarded scientist and intellectual, **Professor Istvan Hargittai**, Editor-in-Chief of "*Structural Chemistry*" has overseen the publication of *Struct. Chem.* **28** (*Issue 5*), October 2017: **Special Issue Honoring Professor Lou Massa: "A Path through Quantum Crystallography"** - Guest Editor: Chérif F. Matta:

https://link.springer.com/journal/11224/28/5/page/1

The Massa special issue collection consists of 33 articles (329 journal pages) written by 83 authors from *Belgium, Canada, China, France, Germany, Greece, Hungary, India, Israel, Italy, Japan, Mexico, Poland, South Africa, Spain, UK,* and *USA*. **It**

includes a congratulatory Editorial by Professor Hargittai and a single-authored tribute article by Nobel Laureate Professor Ada Yonath.

To sum-up QCr, the development of the emerging field of Quantum Crystallography brings the rigor of quantum mechanics to traditional experimental crystallography. This rewards the elegance of drawing from quantum mechanics to expand the field of crystallography. ***In a sense, Quantum Crystallography imposes Nature's quantum mechanical grammar on the electron density derived from X-ray scattering experiments.***

5 Most Significant *(RECENT)* Publications:

- **Massa L,** "*A zigzag path through quantum crystallography*" *Struct. Chem.* **28**, 1293-1296 (2017).
- Polkosnik W, **Massa L**, "*Single determinant* N-*representability and the kernel energy method applied to water clusters*" *J. Comput. Chem.* **39**, 1038-1043 (2018).
- Matta CF, Huang L, **Massa L**, "*Quantum crystallography:* N-*representability big and small*"; *Isr. J. Chem.* **61**, 1-14 (these are not final page numbers, in press) (2021).
  [Invited for special issue of the Journal: *Rosarium Philsophorum*].
- Matta CF, **Massa L**, "*A two projector triple product in quantum crystallography*" *Int. J. Quantum Chem.* **122**, e26838 (2021).
- Polkosnik W, Matta CF, Huang L, Massa L, "*Fast quantum crystallography*", *Int. J. Quantum Chem.* **119**, Article # e25986 (2019).

Awards and Recognitions:

1. Honorary degree, Doctor of Humane Letters, Mount St. Vincent University, 2019
2. Special Issue of *Structural Chemistry* (Springer) Honoring Professor Lou Massa: "A Path through Quantum Crystallography": *Struct. Chem.* 28 (*Issue 5*), October 2017:" - Guest Editor: Chérif F. Matta (including a tribute article by Nobel Laureate Ada Yonath): https://link.springer.com/journal/11224/28/5/page/1
3. Westchester Distinguished Scientist Award, American Chemical Society, 2019
4. Consultant to the permanent Commission of the International Union of Crystallography: Commission on Quantum Crystallography, (Elected in 2021)
5. Honorific mention in Dr. Jerome Karle Nobel Prize biography website: J. Karle, Biographical. Nobel Prize Addendum, April 2006: (https://www.nobelprize.org/prizes/chemistry/1985/karle/biographical/)

6. Distinguished Visiting Professor United States Naval Research Laboratory, 1985-2024.
7. President's Award for Excellence in Research, Hunter College of the City University of New York (CUNY), 1995
8. United States Naval Research Laboratory Berman Award for Outstanding Science Paper 1995

Service to the Community, i.e., highlights of conference/symposia organization, editorial duties, committee service:

1. Keynote address, CECAM Conference on Quantum Crystallography, Current Developments and Future Perspectives", Nancy (France), 19th and 20th of June 2017.
2. Keynote address, Erice School on Quantum Crystallography, Ettore Majorana Research Center, 1-10 June 2018, Erice (Italy).
3. Member International Organizing Committee, Sagamore XIX Conference on Quantum Crystallography, Halifax, 2018
4. Matta, C. F.; Massa, L. (Guest Editors). "*Special Issue: Quantum Crystallography – PART 1 of 2* " Journal of Computational Chemistry, Volume **39**, Issue 17 (June 30, 2018), pp. i, 1013-1075 (2018).
5. Structural Chemistry, Festschrift honoring Professor Lou Massa, 28, No. 5, 1277-1606 (2017)
6. Invited paper, Massa, L. *A zigzag path through quantum crystallography*. *Struct Chem* **28,** 1293–1296 (2017). https://doi.org/10.1007/s11224-017-0960-9

Mentorship of professionals in the field, i.e., highlights of former graduate students and two undergraduate students along with present positions (Selected mentees only)

1. Arnaud Soirat, PhD, Rio Tinto, chief operating officer
2. Maria Flocco, PhD, Vice President, Global Head of Mechanistic and Structural Biology at Astra Zeneca
3. Lulu Huang, PhD, Senior Scientist, US Naval Research Laboratory
4. Carol Frishberg, PhD, Upward Bound Math-Science Project Director, Professor of Chemistry, Ramapo College of New Jersey
5. Martin Goldberg, PhD, Lead Consultant, ValidationQuant
6. Sonjae Wallace PhD, Clinical Professor, Lehman College, CUNY
7. Miriam Rossi, PhD, undergraduate mentee, Mary Landon Sague Endowed Chair & Professor of Chemistry, Vassar College
8. Olga Lavinda, PhD, undergraduate mentee, Chemistry Adjunct Lecturer, Baruch College, CUNY

b. **Publications listed separately: 2 Books, TV series, 237 published papers.**

Books:

- L. Massa, *Science and the Written Word: Science, Technology, and Society*; Oxford University Press: New York (2011).
- L. Massa, L. Huang, C. F. Matta: *Quantum Crystallograph;,* De Gruyter: Berlin (2023).
- L. Massa, *Isabella Karle: Nonpareil of Crystallography* (in progress).

TV-Series (on YouTube):

- *Science and the Written Word: Interviews with Nobel Laureates and Senior Contemporary Scientists and Scholars – City University of New York (CUNY) - TV*. (LINK) https://www.google.ca/search?q=science+and+the+written+word&source=lnms&tbm=vid&sa=X&ved=0ahUKEwi2uNLZgfbVAhVCbxQKHdz_APMQ_AUIDCgD&biw=1090&bih=519&dpr=1.25

Peer Reviewed Research Papers:

[237] Majaess, D.; Seuret, H.; Sullivan, A.; Harriott, T. A.; Morera-Boado, C.; MASSA, L.; Matta, C. F. (2024) "Strengthening the Link Between Fullerenes and a Subset of Diffuse Interstellar Bands"; *Publications of the Astronomical Society of the Pacific*, submitted, in review (ms. PASP-101868).

[236] Majaess, D.; Seuret, H.; Sullivan, A.; Harriott, T. A.; Morera-Boado, C.; MASSA, L.; Matta, C. F. (2024) "Characterizing Functional Groups Within DIB Energy Offsets"; *Publications of the Astronomical Society of the Pacific*, submitted, in review (ms. PASP-101838).

[235] Seuret, H.; Sullivan, A.; Morera-Boado, C.; Harriott, T. A.; Majaess, D.; MASSA, L.; Matta, C. F. (2024) "Vetting Molecular Candidates Linked to the First Diffuse Interstellar Bands Discovered (5760 and 5797 Å)"; *Physical Chemistry Chemical Physics (PCCP)*, submitted, in review.

[234] S.G. Lambrakos, L. Massa, S. Wallace, S. Ramsey,"Dielectric-Response of Energetic Materials based on DFT-Calculated IR Spectra" Canadian Journal of Chemistry, accepted for publication.

[233] MASSA, L.; Matta, C. F. (2024). "The Total Energy from X-Ray Electron Density?",*Journal of Molecular Modeling*, accepted for publication.

[232] Xing, H.; Sullivan, A.; Seuret, H.; Morera-Boado, C.; Harriott, T. A.; Majaess, D.; MASSA, L.; Matta, C. F. (2024) "Extinction Along Sightlines Sampled by the APO Catalog of DIBs"; *Research Notes of the American Astronomical Society (RNAAS)* **8**, Article # 90 (pp.1-3).

[231] K. Ramig, T. Eskaros,T. Islam, O. Lavinda, S. Karimi, L. Massa, and C. Cooksey,
"Thermochromicity in Wool Dyed with 6-Bromoindigo Depends on the Presence and Identity of a Solvent", *Heritage* **2023**, *6*(1), 672-680.

[230] L Massa, P Fahimi, LAM Castanedo, CF Matta, "*In silico approaches andchallenges for quantum chemical calculations on macromolecules"*, In-Silico Approaches to Macromolecular Chemistry, 185-197, (2023).

[229] L Massa, LAM Castanedo, P Fahimi, CF Matta, "*Applications of in silico quantum chemical calculations to large systems: The Kernel Energy Method",* In-Silico Approaches to Macromolecular Chemistry, 199-215, (2023).

[228] S. G. Lambrakos, A. Shabaev, S. Wallace, and L. Massa, *"Micro-to-macroscaling of DFT-calculated IR spectra for spectrum-feature extraction and estimation of dielectric response",* Canadian Journal of Chemistry, 16 May (2023).
[227] S. G. Lambrakos, S. Wallace, A. Shabaev, L. Massa, "*Scalability of DFT-Calculated IR Spectra for Estimating Dielectric Functions,*" Proc. SPIE 12514, Image Sensing Technologies: Materials, Devices, Systems, and Applications X, 125140B (15 June 2023);

doi:10.1117/12.2659073

[226] H. Ajiki, I. Bernal, **L. Massa**, *Acid-based analogs of certain water tetramers: an examination of some crystal structures in the literature* . *Struct Chem* **33**, 1177–1188 (2022).

[225] E. R. Smith, F. M. Smith, T. A. Harriott, D. Majaess, **L. Massa**, and C. F. Matta, *"Novel Correlations between Diffuse Interstellar Bands and Optical Reddening"*, American Astronomical Society, Research Notes of the AAS, Volume 6, Number 4, April 2022

[224] C. F. Matta, **L. Massa**, "*A two projector triple product in quantum crystallography*", **122**, e26838 (2022) [Cover Feature].

[223] C. F. Matta, L. Huang, **L. Massa**, "*Quantum crystallography: N representability big and small*", *Israel Journal of Chemistry* **61**, page numbers to be finalized (in press https://doi.org/10.1002/ijch.202100108) (2021). [Invited to Special Issue: Rosarium Philosophorum].

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

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

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