Alessandro Genoni

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Personal Information

Date of Birth	February 24, 1979
Place of Birth	Magenta (Italy)
Nationality	Italian

Academic Positions

Oct 2011 – Present — **Permanent CNRS Researcher (Chargé de Recherche CNRS - promoted to First Class in October 2015)**.
University of Lorraine - Laboratory of Theoretical Physics and Chemistry (UMR CNRS 7019), Nancy & Metz, France

June 2009 – Sep 2011 — **Post Doctoral Researcher**.
Giorgio Colombo Research Group, CNR - Institute of Chemistry of Molecular Recognition, Milano, Italy

Nov 2006 – May 2009 — **Post Doctoral Researcher**.
Kenneth M. Merz Jr. Research Group, Quantum Theory Project - University of Florida, Gainesville (Florida), USA

Education

September 2018 — **French Habilitation to Direct Research (Habilitation à Diriger des Recherches - HDR)**, *University of Lorraine (Metz, France)*.
Thesis: *Development of Methods in the Framework of the Original Definition of Quantum Crystallography*.

December 2006 — **Ph.D. in Chemistry (major in Theoretical Chemistry)**, *University of Milan (Milano, Italy)*, *full marks and honours*.
Thesis: *Development and Application of Methods Based on Extremely Localized Molecular Orbitals*.
Supervisor: Prof. Maurizio Sironi

July 2003 — **Laurea degree (equivalent to Bachelor and Master degrees) in Chemistry**, *University of Milan (Milano, Italy)*, *full marks and honours (110/110 cum laude)*.
Thesis: *A Novel Approach to Relax Extremely Localized Molecular Orbitals: the ELMO-CI Method*.
Supervisor: Prof. Maurizio Sironi

Other Academic Titles

July 2020 **Italian Habilitation to the position of Associate Professor for the Research Sector 03/A2 "Models and Methodologies for Chemical Sciences" (from July 12, 2020 to July 12, 2029)**, Abilitazione a Professore di Seconda Fascia per il Settore Concorsuale 03/A2 "Modelli e Metodologie per le Scienze Chimiche" (dal 12/07/2020 al 12/07/2029).

July 2020 **Italian Habilitation to the position of Associate Professor for the Research Sector 03/B2 "Chemical Foundations of Technologies" (from July 10, 2020 to July 10, 2029)**, Abilitazione a Professore di Seconda Fascia per il Settore Concorsuale 03/B2 "Fondamenti Chimici delle Tecnologie" (dal 10/07/2020 al 10/07/2029).

Awards & Fellowships

2011 **C. M. Lerici Foundation Scolarship**, *C. M. Lerici Foundation*, Sweden.
Research scholarship to carry out post-doctoral research in the group directed by Roland Lindh (Quantum Chemistry Group, Department of Physical and Analytical Chemistry, Uppsala University).
Declined after getting the CNRS position.

2006 **UNIMI Post-Doctoral Fellowship**, *University of Milan*, Italy.
Research fellowship ("*Borsa di Perfezionamento all'Estero*") sponsored by the University of Milan to allow new Master/Ph.D. laureates to continue their research abroad.
Duration: November 2006 - October 2008.

Grants

2018-2022 **ANR Grant**, *French Research Agency (ANR)*, France.
Project "*QuMacroRef - Original scalable quantum mechanical strategies to refine high-resolution crystallographic structures of macromolecules*" (Grant No. ANR-17-CE29-0005).
Role in the project: Principal Investigator and Coordinator
Duration: February 1, 2018 - January 31, 2022
Financial support: 163,221.56 €

2019-2020 **RFCT Grant**, *Réseau Français de Chimie Théorique (RFCT)*, France.
Grant provided by the *Réseau Français de Chimie Théorique* (RFCT; French Network of Theoretical Chemsitry) for the project "*Development and application of the NCI-ELMO method: from a static to a dynamic picture of non-covalent interactions in macromolecules*" (in collaboration with the group directed by Dr. Julia Contreras-García - Laboratoire de Chimie Théorique, UMR CNRS 7616, Sorbonne University, Paris, France).
Role in the project: Principal Investigator and Coordinator
Duration: May 1, 2019 - March 31, 2020
Financial support: 800.00 €

2018 **GDR SolvATE Grant**, *Groupement de Recherche (GDR) SolvATE*, France.
Travelling grant provided by the *Groupement de Recherche* (GDR) SolvATE for the project "*Construction des librairies moléculaires pour méso-NCI (Construction of molecular libraries for meso-NCI)*".
Role in the project: Co-Principal Investigator together with Dr. Julia Contreras-García (Laboratoire de Chimie Théorique, UMR CNRS 7616, Sorbonne University, Paris, France)
Duration: August 1, 2018 - December 31, 2018
Financial support: 450.00 €

2017-2018 **Institut Jean Barriol Grant**, *University of Lorraine - Jean Barriol Institute*, France.
Research grant provided by the Jean Barriol Institute of the University of Lorraine for the project "*Quantum mechanical models to reconstruct the spin density matrix of magnetic systems*".
Role in the project: Co-Principal Investigator together with Dr. Nicolas Claiser (Laboratoire CRM2, UMR CNRS 7036, Université de Lorraine, Nancy, France)
Duration: May 1, 2017 - December 31, 2018
Financial support: 7,000.00 €

2013-2014 **Institut Jean Barriol Grant**, *University of Lorraine - Jean Barriol Institute*, France.
Research grant provided by the Jean Barriol Institute of the University of Lorraine for the project "*Comparison between Extremely Localized Molecular Orbitals and transferable aspherical pseudoatoms for the reconstruction of polypeptide electron densities*".
Role in the project: Co-Principal Investigator together with Dr. Benoît Guillot (Laboratoire CRM2, UMR CNRS 7036, Université de Lorraine, Nancy, France)
Duration: July 1, 2013 - December 31, 2014
Financial support: 8,000.00 €

2013-2014 **PEPS Mirabelle Grant**, *CNRS & University of Lorraine*, France.
Research grant provided by the CNRS and the University of Lorraine to start the exploratory project "*KiteComb - Electronic kits: original perspectives to model the combustion of second generation biofuels*".
Role in the project: Principal Investigator and Coordinator
Duration: July 3, 2013 - July 2, 2014
Financial support: 20,000.00 €

Current Research Topics

Development of quantum mechanical methods for large systems

- *Construction of libraries of Extremely Localized Molecular Orbitals*
- *Embedding methods based on Extremely Localized Molecular Orbitals*
- *Fast and accurate techniques to detect non-covalent interaction in biosystems*

Development of modern methods of quantum crystallography

- *Determination of wavefunctions from experimental X-ray diffraction data*
- *Extension of the Hirshfeld atom refinement technique to macromolecules*

Main Current Collaborations

- Dr. Nicolas Claiser - Laboratory CRM2, University of Lorraine, Nancy (France)
- Dr. Julia Contreras-García - Laboratory of Theoretical Chemistry, Sorbonne University, Paris (France)
- Prof. Simon Grabowsky - Department of Chemistry and Biochemistry, University of Bern (Switzerland)
- Prof. Benoît Guillot - Laboratory CRM2, University of Lorraine, Nancy (France)
- Prof. Eric Hénon - Institute of Molecular Chemistry of Reims, University of Reims Champagne-Ardenne, Reims (France)
- Prof. Piero Macchi - Department of Chemistry, Materials and Chemical Engineering, Polytechnic University of Milan (Italy)
- Prof. Jacob Overgaard - Department of Chemistry, Aarhus University (Denmark)
- Prof. Maurizio Sironi - Department of Chemistry, University of Milan (Italy)
- Prof. Giancarlo Terraneo - Department of Chemistry, Materials and Chemical Engineering, Polytechnic University of Milan (Italy)

Overall Publication Records *(Web of Science, December 2021)*

- Number of papers in peer-reviewed journals: 59
- Number of book chapters: 3
- Number of citations: 1017
- h-index: 20
- Number of papers as first author and/or corresponding author: 38 (64%)
- Number of papers as single author: 4

- Overall number of oral communications in conferences: 27
- Number of invited oral communications in conferences: 20
- Number of invited seminars in academic institutions: 19

Publications in Peer-Reviewed Journals

- D. Ramírez-Palma, B. Landeros-Rivera, **A. Genoni**, F. Cortés-Guzmán and J. Contreras-García,
  Visualizing Correlation Regions: The Case of the Ammonia Crystal,
  Chemistry-Methods **2**, e202100045 (2022).
- G. Macetti, P. Macchi and **A. Genoni***,
  X-ray restrained extremely localized molecular orbitals for the embedding of quantum mechanical calculations,
  Acta Cryst. B **77**, 695-705 (2021).

- G. Macetti and **A. Genoni***,
  Three-Layer Multiscale Approach Based on Extremely Localized Molecular Orbitals to Investigate Enzyme Reactions,
  J. Phys. Chem. A **125**, 6013-6027 (2021).
- G. Macetti and **A. Genoni***,
  Initial Maximum Overlap Method for Large Systems by the Quantum Mechanics/Extremely Localized Molecular Orbital Embedding Technique,
  J. Chem. Theory Comput. **17**, 4169-4182 (2021).
- G. Macetti and **A. Genoni***,
  Quantum Mechanics / Extremely Localized Molecular Orbital Embedding Technique: Theoretical Foundations and Further Validation,
  Adv. Quantum Chem. **83**, 269-285 (2021).
- G. Macetti, E. K. Wieduwilt and **A. Genoni***,
  QM/ELMO: A Multi-Purpose Fully Quantum Mechanical Embedding Scheme Based on Extremely Localized Molecular Orbitals,
  J. Phys. Chem. A **125**, 2709-2726 (2021). (**Feature Article + Journal Cover**)
- E. K. Wieduwilt, G. Macetti, R. Scatena, P. Macchi and **A. Genoni***,
  Extending Libraries of Extremely Localized Molecular Orbitals to Metal Organic Frameworks: A Preliminary Investigation,
  Crystals **11**, 207 (2021).
- L. A. Malaspina, **A. Genoni** and S. Grabowsky,
  lamaGOET: an Interface for quantum crystallography,
  J. Appl. Cryst. **54**, 987-995 (2021).
- L. A. Malaspina, **A. Genoni**, D. Jayatilaka, M. J. Turner, K. Sugimoto, E. Nishibori and S. Grabowsky,
  The advanced treatment of hydrogen bonding in quantum crystallography,
  J. Appl. Cryst. **54**, 718-729 (2021).
- E. K. Wieduwilt, J.-C. Boisson, G. Terraneo, E. Hénon and **A. Genoni***,
  A Step toward the Quantification of Non-Covalent Interactions in Large Biological Systems: The Independent Gradient Model-Extremely Localized Molecular Orbital Approach,
  J. Chem. Inf. Model. **61**, 795-809 (2021).
- E. K. Wieduwilt, G. Macetti and **A. Genoni***,
  Climbing Jacob's Ladder of Structural Refinement: Introduction of a Localized Molecular Orbital-Based Embedding for Accurate X-ray Determinations of Hydrogen Atom Positions,
  J. Phys. Chem. Lett. **12**, 463-471 (2021).
- S. A. Zein, M.-C. Bordage, Z. Francis, G. Macetti, **A. Genoni**, C. Dal Cappello, W.-G. Shin and S. Incerti,
  Electron transport in DNA bases: An extension of the Geant4-DNA Monte Carlo toolkit,
  Nucl. Instrum. Methods Phys. Res. B **488**, 70-82 (2021).

- F. Kleemiss, O. V. Dolomanov, M. Bodensteiner, N. Peyerimhoff, L. Midgley, L. J. Bourhis, **A. Genoni**, L. A. Malaspina, D. Jayatilaka, J. L. Spencer, F. White, B. Grundkötter-Stock, S. Steinhauer, D. Lentz, H. Puschmann and S. Grabowsky
Accurate Crystal Structures and Chemical Properties from NoSpherA2,
Chem. Sci. **12**, 1675-1692 (2021).
- G. Macetti and **A. Genoni***,
Quantum Mechanics / Extremely Localized Molecular Orbital Embedding Strategy for Excited States: Coupling to Time-Dependent Density Functional Theory and Equation-of-Motion Coupled Cluster,
J. Chem. Theory Comput. **16**, 7490-7506 (2020).
- E. Damgaard-Møller, L. Krause, K. Tolborg, G. Macetti, **A. Genoni** and J. Overgaard
Quantification of the Magnetic Anisotropy of a Single-Molecule Magnet from the Experimental Electron Density,
Angew. Chem. Int. Ed. **59**, 21203-21209 (2020).
- **A. Genoni*** and P. Macchi
Quantum Crystallography in the Last Decade: Developments and Outlooks,
Crystals **10**, 473 (2020).
- G. Macetti, E. K. Wieduwilt, X. Assfeld and **A. Genoni***,
Localized Molecular Orbital-Based Embedding Scheme for Correlated Methods,
J. Chem. Theory Comput. **16**, 3578-3596 (2020).
- D. Franchini, A. Forni, **A. Genoni**, S. Pieraccini, E. Gandini and M. Sironi
The Origin of the σ-Hole in Halogen Atoms: a Valence-Bond Perspective,
ChemistryOpen **9**, 445-450 (2020).
- M. Ernst, **A. Genoni*** and P. Macchi
Analysis of crystal field effects and interactions using X-ray restrained ELMOs,
J. Mol. Struct. **1209**, 127975 (2020).
- E. K. Wieduwilt, G. Macetti, L. A. Malaspina, D. Jayatilaka, S. Grabowsky and **A. Genoni***,
Post-Hartree-Fock methods for Hirshfeld atom refinement: are they necessary? Investigation on a strongly hydrogen-bonded molecular crystal,
J. Mol. Struct. **1209**, 127934 (2020).
- **A. Genoni***,
On the use of the Obara-Saika recurrence relations for the calculation of structure factors in quantum crystallography,
Acta Cryst., Sect. A **76**, 172-179 (2020).
- D. Maiolo, A. Pizzi, A. Gori, L. Gazzera, N. Demitri, **A. Genoni**, F. Baggi, F. Moda, G. Terraneo, F. Baldelli Bombelli, P. Metrangolo and G. Resnati,
Halogenation of the N*-Terminus Tyrosine 10 Promotes Supramolecular Stabilization of the Amyloid-β Sequence 7-12*,
ChemistryOpen **9**, 253-260 (2020).
- C. Gao, **A. Genoni**, S. Gao, A. Soncini, S. Jiang and J. Overgaard,
Direct observation of the asphericity of 4f-electron density and its relation to the magnetic anisotropy axis in single molecule magnets,
Nat. Chem. **12**, 213-219 (2020).

- L. A. Malaspina, E. K. Wieduwilt, J. Bergmann, F. Fleemiss, B. Meyer, M. F. Ruiz-López, R. Pal, E. Hupf, J. Beckmann, R. O. Piltz, A. J. Edwards, S. Grabowsky and **A. Genoni***,
  Fast and Accurate Quantum Crystallography: from Small to Large, form Light to Heavy,
  J. Phys. Chem. Lett. **10**, 6973-6982 (2019).
- M. Fugel, M. V. Ponomarenko, M. F. Hesse, L. A. Malaspina, F. Kleemiss, K. Sugimoto, **A. Genoni**, G.-V. Röschenthaler and S. Grabowsky,
  Complementary bonding analysis of the N-Si interaction in pentacoordinated silicon compounds using quantum crystallography,
  Dalton Trans. **48**, 16330-16339 (2019).
- D. Arias-Olivares, E. K. Wieduwilt, J. Contreras-García and **A. Genoni***,
  NCI-ELMO: a New Method to Quickly and Accurately Detect Non-Covalent Interactions in Biosystems,
  J. Chem. Theory Comput. **15**, 6456-6470 (2019).
- G. Macetti and **A. Genoni***,
  Quantum Mechanics/Extremely Localized Molecular Orbital Method: a Fully Quantum Mechanical Embedding Approach for Macromolecules,
  J. Phys. Chem. A **123**, 9420-9428 (2019).
  (**Selected for the *"Virtual Issue on New Tools and Methods in Physical Chemistry Research"***, see A. B. McCoy, J. Phys. Chem. A **124**, 4323-4324 (2020))
- **A. Genoni***, G. Macetti, D. Franchini, S. Pieraccini and M. Sironi,
  X-ray constrained spin-coupled technique: theoretical details and further assessment of the method,
  Acta Cryst., Sect. A **75**, 778-797 (2019).
- D. Franchini, A. **Genoni**, F. Dapiaggi, S. Pieraccini and M. Sironi
  A valence bond description of the bromine halogen bond,
  Int. J. Quantum Chem. **119**, e25946 (2019).
- M. K. Thomsen, A. Nyvang, J. P. S. Walsh, P. C. Bunting, J. R. Long, F. Neese, M. Atanasov, A. **Genoni** and J. Overgaard
  Insights into Single-Molecule-Magnet Behavior from the Experimental Electron Density of Linear Two-Coordinate Iron Complexes,
  Inorg. Chem. **58**, 3211-3218 (2019).
- B. Meyer and A. **Genoni***,
  Libraries of Extremely Localized molecular Orbitals. 3. Construction and Preliminary Assessment of the New Databanks,
  J. Phys. Chem. A **122**, 8965-8981 (2018).
- **A. Genoni***, D. Franchini, S. Pieraccini and M. Sironi,
  X-ray Constrained Spin-Coupled Wavefunction: a New Tool to Extract Chemical Information from X-ray Diffraction Data,
  Chem. Eur. J. **24**, 15507-15511 (2018). (**Hot Paper**)

- **A. Genoni***, L. Bučinský, N. Claiser, J. Contreras-García, B. Dittrich, P. M. Dominiak, E. Espinosa, C. Gatti, P. Giannozzi, J.-M. Gillet, D. Jayatilaka, P. Macchi, A. Ø. Madsen, L. J. Massa, C. F. Matta, K. M. Merz Jr., P. N. H. Nakashima, H. Ott, U. Ryde, K. Schwarz, M. Sierka and S. Grabowsky,
Quantum Crystallography: Current Developments and Future Perspectives,
Chem. Eur. J. **24**, 10881-10905 (2018). (**Journal Frontispiece**)
- M.-L. Bouressam, B. Meyer, A. Boudier, I. Clarot, P. Leroy, **A. Genoni**, M. F. Ruiz-Lopez, P. Giummelly, P. Liminana, V. Salgues, M. Kouach, C. Perrin-Sarrado, I. Lartaud and F. Dupuis,
In vivo and in silico evaluation of a new nitric oxide donor, S-S'-dinitrosobucillamine,
Nitric Oxide **71**, 32-43 (2017).
- N. Casati, **A. Genoni**, B. Meyer, A. Krawczuk and P. Macchi,
Exploring charge density analysis in crystals at high pressure: data collection, data analysis and advanced modelling,
Acta Cryst., Sect. B **73**, 584-597 (2017).
- A. B. Voufack, N. Claiser, C. Lecomte, S. Pillet, Y. Pontillon, B. Gillon, Z. Yan, J.-M. Gillet, M. Marazzi, **A. Genoni** and M. Souhassou,
When combined X-ray and polarized neutron diffraction data challenge high-level calculations: spin-resolved electron density of an organic radical,
Acta Cryst., Sect. B **73**, 544-549 (2017). (**Journal Cover**)
- **A. Genoni***,
A first-prototype multi-determinant X-ray constrained wavefunction approach: the X-ray constrained extremely localized molecular orbital-valence bond method,
Acta Cryst., Sect. A **73**, 312-316 (2017).
- S. Grabowsky, **A. Genoni*** and H.-B. Bürgi,
Quantum crystallography,
Chem. Sci. **8**, 4159-4176 (2017).
- **A. Genoni***, L. H. R. Dos Santos, B. Meyer and P. Macchi,
Can X-ray constrained Hartree-Fock wavefunctions retrieve electron correlation?,
IUCrJ **4**, 136-146 (2017).
- A. Bertolani, A. Pizzi, L. Pirrie, L. Gazzera, G. Morra, M. Meli, G. Colombo, **A. Genoni**, G. Cavallo, G. Terraneo and P. Metrangolo,
Crystal Structure of the DFNKF Segment of Human Calcitonin Unveils Aromatic Interactions between Phenylalanines,
Chem. Eur. J. **23**, 2051-2058 (2017). (**Journal Cover**)
- B. Meyer, **A. Genoni***, A. Boudier, P. Leroy and M. F. Ruiz-Lopez,
Structure and Stability Studies of Pharmacologiaclly Relevant S-Nitrosothiols: A Theoretical Approach,
J. Phys. Chem. A **120**, 4191-4200 (2016).
- B. Meyer, B. Guillot, M. F. Ruiz-Lopez, C. Jelsch and **A. Genoni***,
Libraries of Extremely Localized Molecular Orbitals. 2. Comparison with the Pseudoatoms Transferability,
J. Chem. Theory Comput. **12**, 1068-1081 (2016).

- B. Meyer, B. Guillot, M. F. Ruiz-Lopez and **A. Genoni***,
  Libraries of Extremely Localized Molecular Orbitals. 1. Model Molecules Approximation and Molecular Orbitals Transferability,
  J. Chem. Theory Comput. **12**, 1052-1067 (2016).
- **A. Genoni*** and B. Meyer,
  X-Ray Constrained Wave Functions: Fundamentals and Effects of the Molecular Orbitals Localization,
  Adv. Quantum Chem. **73**, 333-362 (2016).
- G. Morra, **A. Genoni** and G. Colombo,
  Mechanisms of Differential Allosteric Modulation in Homologous Proteins: Insights from the Analysis of Internal Dynamics and Energetics of PDZ Domains,
  J. Chem. Theory Comput. **10**, 5677-5689 (2014).
- L. H. R. Dos Santos, **A. Genoni*** and P. Macchi,
  Unconstrained and X-ray constrained Extremely Localized Molecular Orbitals: analysis of the reconstructed electron density,
  Acta Cryst., Sect. A **70**, 532-551 (2014). (**Journal Cover**)
- **A. Genoni***,
  X-ray Constrained Extremely Localized Molecular Orbitals: Theory and Critical Assessment of the New Technique,
  J. Chem. Theory Comput. **9**, 3004-3019 (2013).
- **A. Genoni***,
  Molecular Orbitals Strictly Localized on Small Molecular Fragments form X-ray Diffraction Data,
  J. Phys. Chem. Lett. **4**, 1093-1099 (2013).
- **A. Genoni**, M. Pennati, G. Morra, N. Zaffaroni and G. Colombo,
  Ligand selection from the analysis of protein conformational substates: new leads targeting the N-terminal domain of Hsp90,
  RSC Adv. **2**, 4268-4282 (2012).
- **A. Genoni***, G. Morra and G. Colombo,
  Identification of Domains in Protein Structures from the Analysis of Intramolecular Interactions,
  J. Phys. Chem. B **116**, 3331-3343 (2012).
- **A. Genoni**, G. Morra, K. M. Merz Jr. and G. Colombo,
  Computational Study of the Resistance Shown by the Subtype B / HIV-1 Protease to Currently Known Inhibitors,
  Biochemistry **49**, 4283-4295 (2010).
- G. Morra, **A. Genoni**, M. A. C. Neves, K. M. Merz Jr. and G. Colombo,
  Molecular Recognition and Drug-Lead Identification: What Can Molecular Simulations Tell Us?,
  Current Med. Chem. **17**, 25-41 (2010).
- M. Sironi, M. Ghitti, **A. Genoni**, G. Saladino and S. Pieraccini,
  DENPOL: A new program to determine electron densities of polypeptides using extremely localized molecular orbitals,
  J. Mol. Struct. (THEOCHEM) **898**, 8-16 (2009).

- **A. Genoni***, K. M. Merz Jr. and M. Sironi,
  A Hylleraas functional based perturbative technique to relax the extremely localized molecular orbital wavefunction,
  J. Chem. Phys. **129**, 054101 (2008).
- S. Pieraccini, L. Burgi, **A. Genoni**, A. Benedusi and M. Sironi,
  Atomic level description of the protecting effect of osmolytes against thermal denaturation of proteins,
  Chem. Phys. Lettt. **438**, 298-303 (2007).
- M. Sironi, **A. Genoni**, M. Civera, S. Pieraccini, M. Ghitti,
  Extremely Localized Molecular Orbitals: theory and applications,
  Theor. Chem. Acc. **117**, 685-698 (2007).
- **A. Genoni**, M. Ghitti, S. Pieraccini and M. Sironi,
  A novel extremely localized molecular orbitals based technique for the one-electron density matrix computation,
  Chem. Phys. Lett. **415**, 256-260 (2005).
- **A. Genoni**, A. Fornili and M. Sironi,
  Optimal Virtual Orbitals to Relax Wave Functions Built Up with Transferred Extremely Localized Molecular Orbitals,
  J. Comput. Chem. **26**, 827-835 (2005).
- **A. Genoni** and M. Sironi,
  A novel approach to relax extremely localized molecular orbitals: the extremely localized molecular orbital-valence bond method,
  Theor. Chem. Acc. **112**, 254-262 (2004).

Book Chapters

- **A. Genoni*** and D. Jayatilaka,
  X-ray Constrained Wavefunction Analysis with Tonto, in *Complementary Bonding Analysis* (Editor: Simon Grabowsky; ISBN: 978-3-11-066006-7), De Gruyter, Berlin, Germany, 2021; Chapter 11, pp 269-307, DOI: 10.1515/9783110660074-011.
- S. Grabowsky, **A. Genoni**, S. P. Thomas and D. Jayatilaka,
  The Advent of Quantum Crystallography: Form and Structure Factors from Quantum Mechanics for Advanced Structure Refinement and Wavefunction Fitting, in *21st Century Challenges in Chemical Crystallography II - Structural Correlations and Data Interpretation. Structure and Bonding* (Editors: D. Michael P. Mingos and Paul Raithby; Print ISBN: 978-3-030-64746-9; Online ISBN: 978-3-030-64747-6), Springer, Berlin & Heidelberg, Germany, 2021; vol 186, pp 65-144, DOI: 10.1007/430_2020_62.
- G. Morra, **A. Genoni** and G. Colombo,
  Protein Dynamics and Drug Design: the Role of Molecular Simulations, in *Protein-Protein Complexes: Analysis, Modelling and Drug Design* (Editor: Martin Zacharias; ISBN-13: 978-184816-338-6), Imperial College Press, London, UK, 2010; Chapter 13, pp 340-385, DOI: 10.1142/9781848163409_0013.

Papers for a Larger Public

- R. F. Novara, A. **Genoni** and S. Grabowsky,
  What is Quantum Crystallography?,
  Chem. Views, DOI: 10.1002/chemv.201800066 (2018). (**Interview**)

Oral Communications in Conferences

- *Multi-determinant X-ray restrained wavefunction approaches*,
  25th Congress and General Assembly of the International Union of Crystallography,
  Prague (Czech Republic), August 14-22, 2021, **Invited Talk**.
- *Advanced Methods for the Determination of Wavefunctions from Experimental X-ray Diffraction Data*,
  AFC 2021: Colloque 2021 de l'Association Française de Cristallographie,
  Grenoble (France), June 29 - July 2, 2021, **Invited Talk**.
- *QM/ELMO Method: a Fully Quantum Mechanical Embedding Scheme Based on Extremely Localized Molecular Orbitals*,
  WMES 2020: Virtual Warsaw Molecular Electronic Structure Conference,
  Warsaw (Poland), September 1-4, 2020, **Invited Talk**.
- *Quantum Crystallography for Macromolecules: the HAR-ELMO Method*,
  ECM32 - 32nd Meeting of the European Crystallographic Association,
  Vienna (Austria), August 18 -23, 2019.
- *Exploiting Quantum Chemistry to Refine Crystallographic Structures of Proteins and Polypeptides*,
  1st International Charge Density Meeting,
  Göttingen (Germany), July 21-26, 2019, **Invited Talk**.
- *X-ray Constrained Wavefunction Analysis*,
  Tools for Chemical Bonding 2019,
  Bremen (Germany), July 14-19, 2019, **Invited Practical Workshop**.
- *Quantum Crystallography and its application to macromolecules*,
  CECAM School "Simulation of molecular systems for chemistry, materials and biology",
  Lecco (Italy), June 10-14, 2019, **Invited Talk**.
- *HAR-ELMO: a new quantum chemistry-based technique to refine crystallographic structures of proteins*,
  ICCMSE 2019 - Computational Chemistry Symposium,
  Rhodes (Greece), May 1-5, 2019, **Invited Talk**.
- *Exploiting libraries of Extremely Localized Molecular Orbitals to refine protein crystallographic structures*,
  MESM 2018: International Conference on Molecular Electronic Structure,
  Metz (France), August 28-31, 2018.
- *Libraries of Extremely Localized Molecular Orbitals and their coupling to Hirshfeld Atom Refinement*,
  Sagamore 2018,
  Halifax (Nova Scotia, Canada), July 8-13, 2018, **Invited Talk**.

- *Theoretical and X-ray Constrained Extremely Localized Molecular Orbitals*,
  International School of Crystallography - 52nd Course: Quantum Crystallography,
  Erice (Italy), June 1-10, 2018, **Invited Practical Workshop**.
- *Extremely Localized Molecular Orbitals in Quantum Crystallography*,
  International School of Crystallography - 52nd Course: Quantum Crystallography,
  Erice (Italy), June 1-10, 2018, **Invited Lecture**.
- *Coupling Hirshfeld Atom Refinement with libraries of Extremely Localized Molecular Orbitals to refine protein crystallographic structures*,
  ARC Meeting CONTRAST on Engineering Responsive Materials,
  Louvain-la-Neuve (Belgium), March 23, 2018, **Invited Talk**.
- *Quantum Crystallography: original definition and connections to current research developments*,
  26th Annual Meeting of the German Crystallographic Society,
  Essen (Germany), March 5-8, 2018, **Invited Talk**.
- *Libraries of Extremely Localized Molecular Orbitals*,
  24th Congress and General Assembly of the International Union of Crystallography,
  Hyderabad (India), August 21-28, 2017, **Invited Talk**.
- *Quantum Crystllography: Current Developments and Future Perspectives*,
  CECAM Discussion Meeting. Quantum Crystallography: Current Developments and Future Perspectives
  Nancy (France), June 19-20, 2017.
- *Recent Advances in the Determination of "Experimental" Wave Functions*,
  Japan-France-Spain Joint-Symposium on Theoretical and Computational Science of Complex Systems,
  Kyoto (Japan), October 26-28, 2016, **Invited Talk**.
- *Recent Advancements in the Development of X-ray Constrained Wave Function Strategies*,
  ECM30 - 30th Meeting of the European Crystallographic Association,
  Basel (Switzerland), August 28 - September 1, 2016, **Invited Talk**.
- *Searching for "Experimental" Wave Functions: Past, Present and Future*,
  1st Robert F. Stewart School on Electron Density and Related Properties,
  Nancy (France), August 23-26, 2016, **Invited Talk**.
- *Can the X-ray constrained wave function methods extract electron correlation effects on the electron density?*,
  7th European Charge Density Meeting,
  Warsaw (Poland), June 26 - July 1, 2016.
- *X-ray Constrained Wave Functions to Extract Electron Correlation and Crystal Field Effects: Current Investigations and Perspectives*,
  CECAM Workshop: Density- and Response Density-Based Models for Intermolecular Interactions in Molecular Assemblies and in Solids,
  Nancy (France), June 20-23, 2016, **Invited Talk**.
- *New Insights and Perspectives in the Quest for "Experimental" Wave Functions*,
  ICCMSE 2016 - Computational Chemistry Symposium,
  Athens (Greece), March 17-20, 2016, **Invited Talk**

- *X-Ray constrained wave function: new developments and insights*,
  Sagamore XVIII: Conference on Charge, Spin and Momentum Densities,
  Santa Margherita di Pula (Italy), June 7-12, 2015.
- *Looking for "Experimental Wave Functions": Extraction of Extremely Localized Molecular Orbitals from X-Ray Diffraction Data*,
  Molecular Electronic Structure Workshop,
  Amasya (Turkey), September 1-5, 2014, **Invited Talk**.
- *Extracting Extremely Localized Molecular Orbitals from X-Ray Diffraction Data*,
  23rd Congress and General Assembly of the International Union of Crystallography,
  Montreal (Canada), August 5-12, 2014, **Invited Talk**.
- *Extremely Localized Molecular Orbitals from X-Ray Diffraction Data*,
  9th European Conference on Computational Chemistry,
  Sopron (Hungary), September 1-5, 2013.
- *Unraveling the resistance shown by the Subtype B / HIV Protease to currently known inhibitors by means of computational studies*,
  Convegno Nazionale della Divisione di Chimica dei Sistemi Biologici della Società Chimica Italiana: From Molecular Structure to Systems Biology,
  San Vito di Cadore (Italy), September 9-11, 2010.

Other Communications in Conferences

- Co-author and responsible of other 11 oral communications given by supervised Ph.D. students and PostDocs in international or national conferences;
- Co-author of other 5 oral communications given by coworkers in international conferences;
- Main author or co-author of 32 poster presentations given in international or national conferences.

Invited Seminars

- *Development and Application of Quantum Chemistry and Quantum Crystallography Methods*,
  Department of Chemistry, Materials & Chemical Engineering, Polytechnic University of Milan,
  Milan (Italy), November 25, 2021.
- *Development of Computational Methods for Quantum Chemistry and Quantum Crystallography*,
  Department of Chemistry, University of Rome "La Sapienza",
  Rome (Italy), May 24, 2021, **Webinar**.
- *QM/ELMO Method: A Multi-Purpose Embedding Technique Based on Extremely Localized Molecular Orbitals*,
  Theoretical Chemistry Group, Institute of Radical Chemistry, Aix-Marseille University,
  Marseille (France), April 1, 2021, **Webinar**.

- *Development and Application of Methods within the Original Definition of Quantum Crystallography*,
  DESY & University of Hamburg,
  Hamburg (Germany), February 10, 2020.
- *HAR-ELMO: a quantum chemistry-based method to refine crystal structures of polypeptides and proteins*,
  Department of Biology and Biotechnology, Structural Biology Group, University of Pavia,
  Pavia (Italy), December 4, 2019.
- *Libraries of Extremely Localized Molecular Orbitals: new tools to refine protein crystallographic structures?*,
  Department of Chemistry, University of Pavia,
  Pavia (Italy), November 14, 2018.
- *Libraries of Extremely Localized Molecular Orbitals: Preliminary Investigations and Future Perspectives*,
  Institute of Inorganic Chemistry and Crystallography, University of Bremen,
  Bremen (Germany), December 14, 2017.
- *Libraries of Extremely Localized Molecular Orbitals*,
  Department of Chemistry, University of Warsaw,
  Warsaw (Poland), October 27, 2017.
- *X-ray Constrained Wave Function Methods: Recent Studies and New Perspectives*,
  Graduate School of Information Science, Nagoya University,
  Nagoya (Japan), November 1, 2016.
- *New Insights and Perspectives in the Development of X-ray Constrained Wave Function Methods*,
  Dipartimento di Chimica, Università degli Studi di Milano,
  Milano (Italy), September 28, 2016.
- *Looking for X-ray Constrained Wave Functions: the Case of the Extremely Localized Molecular Orbitals*,
  Instituto de Astronomía y Física del Espacio, Universidad de Buenos Aires,
  Buenos Aires (Argentina), November 9, 2015.
- *Extracting Extremely Localized Molecular Orbitals from Experimental X-Ray Diffraction Data*,
  Laboratoire de Chimie Quantique, Université de Strasbourg,
  Strasbourg (France), May 19, 2015.
- *Extemely Localized Molecular Orbitals*,
  Laboratoire SRSMC - UMR CNRS 7565,
  Metz (France), February 28, 2014.
- *Extemely Localized Molecular Orbitals: Past, Present and Future Strategies*,
  Department of Chemistry and Biochemistry, University of Bern,
  Bern (Switzerland), December 12, 2013.
- *Introduction to Quantum Chemistry: from the Basic Approximations to New Methods for the Study of Large Systems*,
  CNR - Istituto di Chmica del Riconoscimento Molecolare,
  Milan (Italy), May 15, 2012.

- *Strategies to investigate energetic and dynamic properties in proteins*,
  Laboratoire SRSMC - UMR CNRS 7565, Université Henry Poincaré,
  Nancy (France), December 2, 2010.
- *Computational study of the resistance shown by the Subtype B / HIV-1 protease to currently known inhibitors*,
  Department of Chemistry - University of South Florida,
  Tampa (Florida, USA), February 17, 2010.
- *Extremely Localized Molecular Orbitals: Methods and Applications*,
  Quantum Theory Project - University of Florida,
  Gainesville (Florida, USA), January 31, 2007.
- *Development and application of methods based on Extremely Localized Molecular Orbitals*,
  Laboratoire SRSMC - UMR CNRS 7565, Université Henry Poincaré,
  Nancy (France), July 5, 2006.

Supervision of Students and PostDocs

PostDocs

- Giovanni Macetti (University of Lorraine, February 2019 - October 2021)
  Main Topic: *Development and application of fully quantum mechanical multi-scale embedding methods*

Ph.D. Students

- Erna Wieduwilt (University of Lorraine, October 2018 - October 2021)
  Thesis: *Quantum mechanics-based methods for the refinement of crystal structures and the analysis of non-covalent interactions* (defended on October 26, 2021)
- Benjamin Meyer (University of Lorraine, October 2013 - October 2016)
  Thesis: *Development and application of methods based on extremely localized molecular orbitals* (defended on October 10, 2016)

Master Students

- Gabriele Favarò (University of Milan, 2006; co-supervisor)
  Thesis: *Rilassamento selettivo di orbitali molecolari estremamente localizzati*

Bachelor Students

- Marco Pitalieri (University of Milan, 2005; co-supervisor)
  Thesis: *Studio delle potenzialità del programma DENPOL attraverso l'applicazione a polileucine e poliglicine*
- Gabriele Favarò (University of Milan, 2004; co-supervisor)
  Thesis: *Ottimizzazione e trasferimento di orbitali molecolari estremamente localizzati*

Teaching Activities (Ordinary Classes)

- Lecturer for the class on *Computational Chemistry* (lectures on Molecular Symmetry) for the Master of Science and Ph.D. in Chemistry (University of Lorraine, 2020/2021; 10 hours).
- Lecturer for the class on *Computational Methods and Molecular Design in Bio-Organic Chemistry* (lectures on quantum chemistry methods) for the Master of Science (*Laurea Magistrale*) in Chemistry (University of Pavia, 2018/2019 & 2019/2020; 8 hours per year).
- Teaching Assistant for the class on *Numerical Analysis and Programming* of the Bachelor of Science (*Laurea Triennale*) in Chemistry (University of Milan, 2004/2005 & 2005/2006; 16 hours per year).
- Teaching Assistant for the class on *Computational Chemistry* of the Bachelor of Science (*Laurea Triennale*) in Chemistry (University of Milan, 2003/2004 & 2004/2005; 16 hours per year).

Teaching Activities (Summer Schools)

- Lecturer at the summer school "*Tools for Chemical Bonding 2019*", (Bremen (Germany), July 14-19, 2019).
- Lecturer at the CECAM school "*Simulation of molecular systems for chemistry, materials and biology*", (Lecco (Italy), June 10-14, 2019).
- Lecturer at the "*International School of Crystallography - 52nd Course: Quantum Crystallography*", (Erice (Italy), June 1-10, 2018).
- Lecturer at the "*1st Robert F. Stewart School on Electron Density and Related Properties*", (Nancy (France), August 23-26, 2016).

Editorial and Reviewer Activities

- Member of the Editorial Board of the journal *Quantum Beam Science* (March 2020 - Present; `https://www.mdpi.com/journal/qubs/editors`);
- Reviewer for international peer-reviewed journals: *Acta Crystallographica A, Acta Crystallographica B, Advances in Quantum Chemistry, Biochemistry, BMC Structural Biology, Bioorganic & Medicinal Chemistry Letters, Chemistry - A European Journal, Chemistry (MDPI), Computational and Theoretical Chemistry, Crystals, Inorganic Chemistry, International Journal of Quantum Chemistry, Journal of Alloys and Compounds, Journal of Chemical Information and Modeling, Journal of Chemical Theory and Computation, Journal of Computational Chemistry, Journal of Molecular Modelling, Science Advances, The Journal of Chemical Physics, The Journal of Physical Chemistry A/B/C/Letters*;
- Reviewer of research projects for national research agencies;
- Reviewer of computational research projects for national and international High-Performance Computing Centers;
- Reviewer and jury member for Master and Ph.D. theses.

- Official reviewer appointed by the doctoral schools *SESAMES* and *C2MP* of the University of Lorraine for the evaluation *in itinere* (i.e., after the first and second years) of Ph.D. theses.

Organization of Conferences, Workshops and Schools

- Current member of the Scientific Program committee for the "*33th Meeting of the European Crystallographic Association*" (Versailles (France), August 23-27, 2022).
- Co-organizer and Co-Chair of the CECAM Workshop "*Second Discussion Meeting on Quantum Crystallography: Expectations and Reality*" (Online Meeting, September 9-12, 2021).
- Chairman and co-organizer of one session of "*QCrOM2020: Quantum Crystallography Online Meeting 2020*" (Online Meeting, August 26-29, 2020).
- Member of the local organizing committee of the conference "*COPIAMC 2109: 20th International Symposium on Correlation, Polarization and Ionization in Atomic and Molecular Collisions*" (Metz (France), August 1-3, 2019).
- Member of the scientific and organizing committee of the workshop "*TCB 2019: Tools for Chemical Bonding*" (Bremen (Germany), July 14-19, 2019).
- Member of the local organizing committee of the conference "*MESM 2018: International Conference on Molecular Electronic Structure*" (Metz (France), August 28-31, 2018).
- Main organizer and Co-Chair of the CECAM Discussion Meeting "*Quantum Crystallography: Current Developments and Future Perspectives*" (Nancy (France), June 19-20, 2017).
- Chairman and co-organizer of the microsymposium "*Beyond the mulltipolar refinement*" in the framework of the "*30th Meeting of the European Crystallographic Association*" (Basel (Switzerland), August 28 - September 1, 2016).
- Member of the local organizing committee of the conference "*MPS 2014: International Conference on Many Particle Spectroscopy of Atoms, Molecules, Clusters and Surfaces*" (Metz (France), July 15-18, 2014).

Administrative Appointments

- Member of the Scientific/Directive Council of the *Laboratory of Theoretical Physics and Chemistry* of the University of Lorraine (September 2020 - Present).
- Responsible of the "Numerical and Theoretical Development" research axis of the *Laboratory of Theoretical Physics and Chemistry* of the University of Lorraine (April 2020 - Present).
- Elected Secretary of the *Special Interest Group 2* (SIG2) on "Quantum Crystallography" of the *European Crystallographic Association* (August 2018 - Present).
- Responsible of the scientific communication for the *Laboratory of Theoretical Physics and Chemistry* of the University of Lorraine (June 2018 - Present).

- Member of the working group for the creation of the new *Laboratory of Theoretical Physics and Chemistry* of the University of Lorraine (October 2015 - October 2016).
- Ph.D. member of the Council of the *Department of Physical Chemistry and Electrochemistry* of the University of Milan (December 2003 - October 2006).

Other Skills

Computational Skills

- Knowledge of operating systems: MacOS, Windows and Linux.
- Knowledge of programming languages: Fortran 77 (advanced), Fortran 90 (advanced), Bash (intermediate).
- Development of codes for scientific calculation in Fortran 77 and Fortran 90 and their inclusion in optimized packages for quantum chemistry calculations (particularly Gaussian, GAMESS-UK and GAMESS-UK).
- Use of common packages and programs for quantum chemistry calculations and quantum chemical topological analyses: Gaussian, GAMESS-US, GAMESS-UK, Tonto, AIMAll, NCI, IGM.
- Use of suite of programs to perform Molecular Dynamics simulations and relative analyses: Amber and Gromacs.
- Use of software for molecular visualisation: GaussView, Mercury, gOpenMol, VMD, Vesta and SwissPDBViever.
- Other software: Matlab, Octave, XMGrace, LaTEX, Microsoft Office, Keynote.

Languages Skills

- Italian: Native speaker
- English: Fluent (listening, speaking, reading and writing)
- French: Fluent (listening, speaking, reading and writing)

Metz (France). February 7, 2022