

# Alessandro Genoni

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/4076809/publications.pdf>

Version: 2024-02-01

74  
papers

1,727  
citations

218677

26  
h-index

302126

39  
g-index

79  
all docs

79  
docs citations

79  
times ranked

995  
citing authors

#	ARTICLE	IF	CITATIONS
1	Accurate crystal structures and chemical properties from NoSpherA2. <i>Chemical Science</i> , 2021, 12, 1675-1692.	7.4	147
2	Quantum crystallography. <i>Chemical Science</i> , 2017, 8, 4159-4176.	7.4	112
3	Quantum Crystallography: Current Developments and Future Perspectives. <i>Chemistry - A European Journal</i> , 2018, 24, 10881-10905.	3.3	108
4	Libraries of Extremely Localized Molecular Orbitals. 1. Model Molecules Approximation and Molecular Orbitals Transferability. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1052-1067.	5.3	64
5	Extremely localized molecular orbitals: theory and applications. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 685-698.	1.4	60
6	Libraries of Extremely Localized Molecular Orbitals. 3. Construction and Preliminary Assessment of the New Databanks. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8965-8981.	2.5	51
7	Observation of the asphericity of 4f-electron density and its relation to the magnetic anisotropy axis in single-molecule magnets. <i>Nature Chemistry</i> , 2020, 12, 213-219.	13.6	50
8	Libraries of Extremely Localized Molecular Orbitals. 2. Comparison with the Pseudoatoms Transferability. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1068-1081.	5.3	48
9	Fast and Accurate Quantum Crystallography: From Small to Large, from Light to Heavy. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6973-6982.	4.6	48
10	Can X-ray constrained Hartree-Fock wavefunctions retrieve electron correlation?. <i>IUCr</i> , 2017, 4, 136-146.	2.2	44
11	Mechanisms of Differential Allosteric Modulation in Homologous Proteins: Insights from the Analysis of Internal Dynamics and Energetics of PDZ Domains. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5677-5689.	5.3	43
12	X-ray Constrained Extremely Localized Molecular Orbitals: Theory and Critical Assessment of the New Technique. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3004-3019.	5.3	42
13	Exploring charge density analysis in crystals at high pressure: data collection, data analysis and advanced modelling. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2017, 73, 584-597.	1.1	42
14	Identification of Domains in Protein Structures from the Analysis of Intramolecular Interactions. <i>Journal of Physical Chemistry B</i> , 2012, 116, 3331-3343.	2.6	41
15	Molecular Recognition and Drug-Lead Identification: What Can Molecular Simulations Tell Us?. <i>Current Medicinal Chemistry</i> , 2010, 17, 25-41.	2.4	39
16	Unconstrained and X-ray constrained extremely localized molecular orbitals: analysis of the reconstructed electron density. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2014, 70, 532-551.	0.1	36
17	A novel extremely localized molecular orbitals based technique for the one-electron density matrix computation. <i>Chemical Physics Letters</i> , 2005, 415, 256-260.	2.6	35
18	Molecular Orbitals Strictly Localized on Small Molecular Fragments from X-ray Diffraction Data. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1093-1099.	4.6	35

#	ARTICLE	IF	CITATIONS
19	Quantum Mechanics/Extremely Localized Molecular Orbital Method: A Fully Quantum Mechanical Embedding Approach for Macromolecules. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9420-9428.	2.5	32
20	A novel approach to relax extremely localized molecular orbitals: the extremely localized molecular orbital-valence bond method. <i>Theoretical Chemistry Accounts</i> , 2004, 112, 254.	1.4	31
21	X-Ray Constrained Wave Functions. <i>Advances in Quantum Chemistry</i> , 2016, 73, 333-362.	0.8	31
22	Optimal virtual orbitals to relax wave functions built up with transferred extremely localized molecular orbitals. <i>Journal of Computational Chemistry</i> , 2005, 26, 827-835.	3.3	30
23	Crystal Structure of the DFNKF Segment of Human Calcitonin Unveils Aromatic Interactions between Phenylalanines. <i>Chemistry - A European Journal</i> , 2017, 23, 2051-2058.	3.3	28
24	Insights into Single-Molecule-Magnet Behavior from the Experimental Electron Density of Linear Two-Coordinate Iron Complexes. <i>Inorganic Chemistry</i> , 2019, 58, 3211-3218.	4.0	28
25	Quantum Crystallography in the Last Decade: Developments and Outlooks. <i>Crystals</i> , 2020, 10, 473.	2.2	28
26	DENPOL: A new program to determine electron densities of polypeptides using extremely localized molecular orbitals. <i>Computational and Theoretical Chemistry</i> , 2009, 898, 8-16.	1.5	27
27	A first-prototype multi-determinant X-ray constrained wavefunction approach: the X-ray constrained extremely localized molecular orbital-valence bond method. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2017, 73, 312-316.	0.1	26
28	X-ray Constrained Spin-Coupled Wavefunction: a New Tool to Extract Chemical Information from X-ray Diffraction Data. <i>Chemistry - A European Journal</i> , 2018, 24, 15507-15511.	3.3	25
29	Quantum Mechanics/Extremely Localized Molecular Orbital Embedding Strategy for Excited States: Coupling to Time-Dependent Density Functional Theory and Equation-of-Motion Coupled Cluster. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7490-7506.	5.3	23
30	Climbing Jacob's Ladder of Structural Refinement: Introduction of a Localized Molecular Orbital-Based Embedding for Accurate X-ray Determinations of Hydrogen Atom Positions. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 463-471.	4.6	23
31	Post-Hartree-Fock methods for Hirshfeld atom refinement: are they necessary? Investigation of a strongly hydrogen-bonded molecular crystal. <i>Journal of Molecular Structure</i> , 2020, 1209, 127934.	3.6	22
32	NCI-ELMO: A New Method To Quickly and Accurately Detect Noncovalent Interactions in Biosystems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6456-6470.	5.3	21
33	Analysis of crystal field effects and interactions using X-ray restrained ELMOs. <i>Journal of Molecular Structure</i> , 2020, 1209, 127975.	3.6	21
34	Computational Study of the Resistance Shown by the Subtype B/HIV-1 Protease to Currently Known Inhibitors. <i>Biochemistry</i> , 2010, 49, 4283-4295.	2.5	18
35	Structure and Stability Studies of Pharmacologically Relevant <i>S</i> -Nitrosothiols: A Theoretical Approach. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4191-4200.	2.5	18
36	Localized Molecular Orbital-Based Embedding Scheme for Correlated Methods. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3578-3596.	5.3	18

#	ARTICLE	IF	CITATIONS
37	X-ray constrained spin-coupled technique: theoretical details and further assessment of the method. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2019, 75, 778-797.	0.1	17
38	The Advent of Quantum Crystallography: Form and Structure Factors from Quantum Mechanics for Advanced Structure Refinement and Wavefunction Fitting. <i>Structure and Bonding</i> , 2020, , 65-144.	1.0	17
39	Electron transport in DNA bases: An extension of the Geant4-DNA Monte Carlo toolkit. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 2021, 488, 70-82.	1.4	14
40	A Hylleraas functional based perturbative technique to relax the extremely localized molecular orbital wavefunction. <i>Journal of Chemical Physics</i> , 2008, 129, 054101.	3.0	13
41	When combined X-ray and polarized neutron diffraction data challenge high-level calculations: spin-resolved electron density of an organic radical. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2017, 73, 544-549.	1.1	13
42	A Step toward the Quantification of Noncovalent Interactions in Large Biological Systems: The Independent Gradient Model-Extremely Localized Molecular Orbital Approach. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 795-809.	5.4	13
43	Quantification of the Magnetic Anisotropy of a Single Molecule Magnet from the Experimental Electron Density. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 21203-21209.	13.8	11
44	The advanced treatment of hydrogen bonding in quantum crystallography. <i>Journal of Applied Crystallography</i> , 2021, 54, 718-729.	4.5	11
45	lamaGOET: an interface for quantum crystallography. <i>Journal of Applied Crystallography</i> , 2021, 54, 987-995.	4.5	10
46	Initial Maximum Overlap Method for Large Systems by the Quantum Mechanics/Extremely Localized Molecular Orbital Embedding Technique. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4169-4182.	5.3	10
47	Atomic level description of the protecting effect of osmolytes against thermal denaturation of proteins. <i>Chemical Physics Letters</i> , 2007, 438, 298-303.	2.6	9
48	QM/ELMO: A Multi-Purpose Fully Quantum Mechanical Embedding Scheme Based on Extremely Localized Molecular Orbitals. <i>Journal of Physical Chemistry A</i> , 2021, 125, 2709-2726.	2.5	9
49	Complementary bonding analysis of the N-Si interaction in pentacoordinated silicon compounds using quantum crystallography. <i>Dalton Transactions</i> , 2019, 48, 16330-16339.	3.3	8
50	Ligand selection from the analysis of protein conformational substates: new leads targeting the N-terminal domain of Hsp90. <i>RSC Advances</i> , 2012, 2, 4268.	3.6	7
51	What Is Quantum Crystallography?. <i>ChemistryViews</i> , 0, , .	0.0	7
52	On the use of the Obara-Saika recurrence relations for the calculation of structure factors in quantum crystallography. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2020, 76, 172-179.	0.1	7
53	On the termination of the X-ray constrained wavefunction procedure: reformulation of the method for an unequivocal determination of $\bar{\rho}$ . <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2022, 78, 302-308.	0.1	7
54	Halogenation of the N-Terminus Tyrosine 10 Promotes Supramolecular Stabilization of the Amyloid $\beta$ Sequence 7-12. <i>ChemistryOpen</i> , 2020, 9, 253-260.	1.9	6

#	ARTICLE	IF	CITATIONS
55	X-ray restrained extremely localized molecular orbitals for the embedding of quantum mechanical calculations. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2021, 77, 695-705.	1.1	6
56	Three-Layer Multiscale Approach Based on Extremely Localized Molecular Orbitals to Investigate Enzyme Reactions. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6013-6027.	2.5	5
57	A valence bond description of the bromine halogen bond. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25946.	2.0	4
58	The Origin of the "Hole" in Halogen Atoms: a Valence Bond Perspective. <i>ChemistryOpen</i> , 2020, 9, 445-450.	1.9	4
59	Extending Libraries of Extremely Localized Molecular Orbitals to Metal Organic Frameworks: A Preliminary Investigation. <i>Crystals</i> , 2021, 11, 207.	2.2	4
60	Remarks on X-ray constrained/restrained wavefunction fitting. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2022, 78, 298-304.	1.1	4
61	In vivo and in silico evaluation of a new nitric oxide donor, S,S'-dinitrosobucillamine. <i>Nitric Oxide - Biology and Chemistry</i> , 2017, 71, 32-43.	2.7	3
62	Quantum mechanics/extremely localized molecular orbital embedding technique: Theoretical foundations and further validation. <i>Advances in Quantum Chemistry</i> , 2021, 83, 269-285.	0.8	3
63	Quantification of the Magnetic Anisotropy of a Single-Molecule Magnet from the Experimental Electron Density. <i>Angewandte Chemie</i> , 2020, 132, 21389-21395.	2.0	2
64	Visualizing Correlation Regions: The Case of the Ammonia Crystal. <i>Chemistry Methods</i> , 0, , .	3.8	2
65	Recent advancements in the development of X-ray constrained wave function strategies. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2016, 72, s163-s164.	0.1	2
66	Frontispiece: Quantum Crystallography: Current Developments and Future Perspectives. <i>Chemistry - A European Journal</i> , 2018, 24, .	3.3	1
67	Extracting Extremely Localized Molecular Orbitals from X-ray Diffraction Data. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2014, 70, C284-C284.	0.1	1
68	Libraries of extremely localized molecular orbitals. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2017, 73, C1435-C1435.	0.1	1
69	Joint refinement of spin and charge densities of organic radicals. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2017, 73, C1364-C1364.	0.1	0
70	Ionization of NH <sub>3</sub> by Electron and Photon Impact. <i>Journal of Physics: Conference Series</i> , 2017, 875, 062029.	0.4	0
71	Probability densities in different spaces: when multipolar-atom model is just not enough. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2016, 72, s85-s85.	0.1	0
72	HAR-ELMO: a new quantum mechanics-based method to refine crystallographic structures of proteins. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2018, 74, e230-e230.	0.1	0

#	ARTICLE	IF	CITATIONS
73	Quantum crystallography for macromolecules: the HAR-ELMO method. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, e354-e354.	0.1	0
74	Insights into the origin of magnetic anisotropy in linear iron complexes from the experimental electron density. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, e370-e370.	0.1	0