Alessandro Genoni

List of Publications by Year
in descending order

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74	1,727	218677	302126
papers	citations	26 h-index	39 g-index

79	79	79	995
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Remarks on X-ray constrained/restrained wavefunction fitting. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2022, 78, 298-304.	1.1	4
2	On the termination of the X-ray constrained wavefunction procedure: reformulation of the method for an unequivocal determination of Î». Acta Crystallographica Section A: Foundations and Advances, 2022, 78, 302-308.	0.1	7
3	Accurate crystal structures and chemical properties from NoSpherA2. Chemical Science, 2021, 12, 1675-1692.	7.4	147
4	A Step toward the Quantification of Noncovalent Interactions in Large Biological Systems: The Independent Gradient Model-Extremely Localized Molecular Orbital Approach. Journal of Chemical Information and Modeling, 2021, 61, 795-809.	5.4	13
5	Electron transport in DNA bases: An extension of the Geant4-DNA Monte Carlo toolkit. Nuclear Instruments & Methods in Physics Research B, 2021, 488, 70-82.	1.4	14
6	Extending Libraries of Extremely Localized Molecular Orbitals to Metal Organic Frameworks: A Preliminary Investigation. Crystals, 2021, 11, 207.	2.2	4
7	QM/ELMO: A Multi-Purpose Fully Quantum Mechanical Embedding Scheme Based on Extremely Localized Molecular Orbitals. Journal of Physical Chemistry A, 2021, 125, 2709-2726.	2.5	9
8	lamaGOET: an interface for quantum crystallography. Journal of Applied Crystallography, 2021, 54, 987-995.	4.5	10
9	The advanced treatment of hydrogen bonding in quantum crystallography. Journal of Applied Crystallography, 2021, 54, 718-729.	4.5	11
10	Three-Layer Multiscale Approach Based on Extremely Localized Molecular Orbitals to Investigate Enzyme Reactions. Journal of Physical Chemistry A, 2021, 125, 6013-6027.	2.5	5
11	Initial Maximum Overlap Method for Large Systems by the Quantum Mechanics/Extremely Localized Molecular Orbital Embedding Technique. Journal of Chemical Theory and Computation, 2021, 17, 4169-4182.	5.3	10
12	X-ray restrained extremely localized molecular orbitals for the embedding of quantum mechanical calculations. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2021, 77, 695-705.	1.1	6
13	Quantum mechanics/extremely localized molecular orbital embedding technique: Theoretical foundations and further validation. Advances in Quantum Chemistry, 2021, 83, 269-285.	0.8	3
14	Climbing Jacobâ€™s Ladder of Structural Refinement: Introduction of a Localized Molecular Orbital-Based Embedding for Accurate X-ray Determinations of Hydrogen Atom Positions. Journal of Physical Chemistry Letters, 2021, 12, 463-471.	4.6	23
15	Observation of the asphericity of 4f-electron density and its relation to the magnetic anisotropy axis in single-molecule magnets. Nature Chemistry, 2020, 12, 213-219.	13.6	50
16	Quantum Mechanics/Extremely Localized Molecular Orbital Embedding Strategy for Excited States: Coupling to Time-Dependent Density Functional Theory and Equation-of-Motion Coupled Cluster. Journal of Chemical Theory and Computation, 2020, 16, 7490-7506.	5.3	23
17	Quantification of the Magnetic Anisotropy of a Singleâ€Molecule Magnet from the Experimental Electron Density. Angewandte Chemie, 2020, 132, 21389-21395.	2.0	2
18	Quantification of the Magnetic Anisotropy of a Singleâ€Molecule Magnet from the Experimental Electron Density. Angewandte Chemie - International Edition, 2020, 59, 21203-21209.	13.8	11

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19	The Advent of Quantum Crystallography: Form and Structure Factors from Quantum Mechanics for Advanced Structure Refinement and Wavefunction Fitting. Structure and Bonding, 2020, , 65-144.	1.0	17
20	Localized Molecular Orbital-Based Embedding Scheme for Correlated Methods. Journal of Chemical Theory and Computation, 2020, 16, 3578-3596.	5.3	18
21	Quantum Crystallography in the Last Decade: Developments and Outlooks. Crystals, 2020, 10, 473.	2.2	28
22	Analysis of crystal field effects and interactions using X-ray restrained ELMOs. Journal of Molecular Structure, 2020, 1209, 127975.	3.6	21
23	Halogenation of the N â€Terminus Tyrosine 10 Promotes Supramolecular Stabilization of the Amyloidâ€Î² Sequence 7â€“12. ChemistryOpen, 2020, 9, 253-260.	1.9	6
24	Post-Hartree-Fock methods for Hirshfeld atom refinement: are they necessary? Investigation of a strongly hydrogen-bonded molecular crystal. Journal of Molecular Structure, 2020, 1209, 127934.	3.6	22
25	The Origin of the Ïƒâ€Hole in Halogen Atoms: a Valence Bond Perspective. ChemistryOpen, 2020, 9, 445-450.	1.9	4
26	On the use of the Obaraâ€“Saika recurrence relations for the calculation of structure factors in quantum crystallography. Acta Crystallographica Section A: Foundations and Advances, 2020, 76, 172-179.	0.1	7
27	Fast and Accurate Quantum Crystallography: From Small to Large, from Light to Heavy. Journal of Physical Chemistry Letters, 2019, 10, 6973-6982.	4.6	48
28	X-ray constrained spin-coupled technique: theoretical details and further assessment of the method. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 778-797.	0.1	17
29	Quantum Mechanics/Extremely Localized Molecular Orbital Method: A Fully Quantum Mechanical Embedding Approach for Macromolecules. Journal of Physical Chemistry A, 2019, 123, 9420-9428.	2.5	32
30	NCI-ELMO: A New Method To Quickly and Accurately Detect Noncovalent Interactions in Biosystems. Journal of Chemical Theory and Computation, 2019, 15, 6456-6470.	5.3	21
31	A valence bond description of the bromine halogen bond. International Journal of Quantum Chemistry, 2019, 119, e25946.	2.0	4
32	Insights into Single-Molecule-Magnet Behavior from the Experimental Electron Density of Linear Two-Coordinate Iron Complexes. Inorganic Chemistry, 2019, 58, 3211-3218.	4.0	28
33	Complementary bonding analysis of the Nâ€“Si interaction in pentacoordinated silicon compounds using quantum crystallography. Dalton Transactions, 2019, 48, 16330-16339.	3.3	8
34	Quantum crystallography for macromolecules: the HAR-ELMO method. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, e354-e354.	0.1	0
35	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
36	Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, 10881-10905.	3.3	108

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37	Xâ€ray Constrained Spinâ€Coupled Wavefunction: a New Tool to Extract Chemical Information from Xâ€ray Diffraction Data. Chemistry - A European Journal, 2018, 24, 15507-15511.	3.3	25
38	Libraries of Extremely Localized Molecular Orbitals. 3. Construction and Preliminary Assessment of the New Databanks. Journal of Physical Chemistry A, 2018, 122, 8965-8981.	2.5	51
39	Frontispiece: Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, .	3.3	1
40	HAR-ELMO: a new quantum mechanics-based method to refine crystallographic structures of proteins. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e230-e230.	0.1	0
41	Can X-ray constrained Hartreeâ€“Fock wavefunctions retrieve electron correlation?. IUCrJ, 2017, 4, 136-146.	2.2	44
42	Quantum crystallography. Chemical Science, 2017, 8, 4159-4176.	7.4	112
43	In vivo and in silico evaluation of a new nitric oxide donor, S,Sâ€² -dinitrosobucillamine. Nitric Oxide - Biology and Chemistry, 2017, 71, 32-43.	2.7	3
44	A first-prototype multi-determinant X-ray constrained wavefunction approach: the X-ray constrained extremely localized molecular orbitalâ€“valence bond method. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, 312-316.	0.1	26
45	Crystal Structure of the DFNKF Segment of Human Calcitonin Unveils Aromatic Interactions between Phenylalanines. Chemistry - A European Journal, 2017, 23, 2051-2058.	3.3	28
46	Joint refinement of spin and charge densities of organic radicals. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C1364-C1364.	0.1	0
47	When combined X-ray and polarized neutron diffraction data challenge high-level calculations: spin-resolved electron density of an organic radical. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 544-549.	1.1	13
48	Exploring charge density analysis in crystals at high pressure: data collection, data analysis and advanced modelling. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 584-597.	1.1	42
49	Ionization of NH₃by Electron and Photon Impact. Journal of Physics: Conference Series, 2017, 875, 062029.	0.4	0
50	Libraries of extremely localized molecular orbitals. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C1435-C1435.	0.1	1
51	X-Ray Constrained Wave Functions. Advances in Quantum Chemistry, 2016, 73, 333-362.	0.8	31
52	Structure and Stability Studies of Pharmacologically Relevant S-Nitrosothiols: A Theoretical Approach. Journal of Physical Chemistry A, 2016, 120, 4191-4200.	2.5	18
53	Libraries of Extremely Localized Molecular Orbitals. 1. Model Molecules Approximation and Molecular Orbitals Transferability. Journal of Chemical Theory and Computation, 2016, 12, 1052-1067.	5.3	64
54	Libraries of Extremely Localized Molecular Orbitals. 2. Comparison with the Pseudoatoms Transferability. Journal of Chemical Theory and Computation, 2016, 12, 1068-1081.	5.3	48

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55	Recent advancements in the development of X-ray constrained wave function strategies. Acta Crystallographica Section A: Foundations and Advances, 2016, 72, s163-s164.	0.1	2
56	Probability densities in different spaces: when multipolar-atom model is just not enough. Acta Crystallographica Section A: Foundations and Advances, 2016, 72, s85-s85.	0.1	0
57	Unconstrained and X-ray constrained extremely localized molecular orbitals: analysis of the reconstructed electron density. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, 532-551.	0.1	36
58	Mechanisms of Differential Allosteric Modulation in Homologous Proteins: Insights from the Analysis of Internal Dynamics and Energetics of PDZ Domains. Journal of Chemical Theory and Computation, 2014, 10, 5677-5689.	5.3	43
59	Extracting Extremely Localized Molecular Orbitals from X-ray Diffraction Data. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C284-C284.	0.1	1
60	Molecular Orbitals Strictly Localized on Small Molecular Fragments from X-ray Diffraction Data. Journal of Physical Chemistry Letters, 2013, 4, 1093-1099.	4.6	35
61	X-ray Constrained Extremely Localized Molecular Orbitals: Theory and Critical Assessment of the New Technique. Journal of Chemical Theory and Computation, 2013, 9, 3004-3019.	5.3	42
62	Ligand selection from the analysis of protein conformational substates: new leads targeting the N-terminal domain of Hsp90. RSC Advances, 2012, 2, 4268.	3.6	7
63	Identification of Domains in Protein Structures from the Analysis of Intramolecular Interactions. Journal of Physical Chemistry B, 2012, 116, 3331-3343.	2.6	41
64	Molecular Recognition and Drug-Lead Identification: What Can Molecular Simulations Tell Us?. Current Medicinal Chemistry, 2010, 17, 25-41.	2.4	39
65	Computational Study of the Resistance Shown by the Subtype B/HIV-1 Protease to Currently Known Inhibitors. Biochemistry, 2010, 49, 4283-4295.	2.5	18
66	DENPOL: A new program to determine electron densities of polypeptides using extremely localized molecular orbitals. Computational and Theoretical Chemistry, 2009, 898, 8-16.	1.5	27
67	A Hylleraas functional based perturbative technique to relax the extremely localized molecular orbital wavefunction. Journal of Chemical Physics, 2008, 129, 054101.	3.0	13
68	Atomic level description of the protecting effect of osmolytes against thermal denaturation of proteins. Chemical Physics Letters, 2007, 438, 298-303.	2.6	9
69	Extremely localized molecular orbitals: theory and applications. Theoretical Chemistry Accounts, 2007, 117, 685-698.	1.4	60
70	A novel extremely localized molecular orbitals based technique for the one-electron density matrix computation. Chemical Physics Letters, 2005, 415, 256-260.	2.6	35
71	Optimal virtual orbitals to relax wave functions built up with transferred extremely localized molecular orbitals. Journal of Computational Chemistry, 2005, 26, 827-835.	3.3	30
72	A novel approach to relax extremely localized molecular orbitals: the extremely localized molecular orbital?valence bond method. Theoretical Chemistry Accounts, 2004, 112, 254.	1.4	31

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73	Visualizing Correlation Regions: The Case of the Ammonia Crystal. Chemistry Methods, 0, , .	3.8	2
74	What Is Quantum Crystallography?. ChemistryViews, 0, , .	0.0	7