Loriano Storchi

List of Publications by Year
in descending order

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75 papers	1,776 citations	393982 19 h-index	276539 41 g-index
81 all docs	81 docs citations	81 times ranked	3905 citing authors

#	Article	IF	Citations
1	Scientific objectives of Einstein Telescope. Classical and Quantum Gravity, 2012, 29, 124013.	1.5	355
2	New and Original pK_a Prediction Method Using Grid Molecular Interaction Fields. Journal of Chemical Information and Modeling, 2007, 47, 2172-2181.	2.5	277
3	Tautomer Enumeration and Stability Prediction for Virtual Screening on Large Chemical Databases. Journal of Chemical Information and Modeling, 2009, 49, 68-75.	2.5	119
4	Extending pKa prediction accuracy: High-throughput pKa measurements to understand pKa modulation of new chemical series. European Journal of Medicinal Chemistry, 2010, 45, 4270-4279.	2.6	107
5	Inherent electronic trap states in TiO2 nanocrystals: effect of saturation and sintering. Energy and Environmental Science, 2013, 6, 1221.	15.6	76
6	In silico pK_a Prediction and ADME Profiling. Chemistry and Biodiversity, 2009, 6, 1812-1821.	1.0	70
7	Recent advances and perspectives in four-component Diracâ€“Kohnâ€“Sham calculations. Physical Chemistry Chemical Physics, 2011, 13, 12368.	1.3	59
8	Molecular photoionization cross sections by Stieltjesâ€“Chebyshev moment theory applied to Lanczos pseudospectra. Journal of Chemical Physics, 2009, 130, 064104.	1.2	37
9	Complete valence double photoionization of SF6. Journal of Chemical Physics, 2005, 122, 144309.	1.2	29
10	The Auger spectroscopy of pyrimidine and halogen-substituted pyrimidines. Journal of Chemical Physics, 2008, 129, 154309.	1.2	28
11	An Efficient Parallel All-Electron Four-Component Diracâ^'Kohnâ^'Sham Program Using a Distributed Matrix Approach. Journal of Chemical Theory and Computation, 2010, 6, 384-394.	2.3	27
12	An experimental and theoretical study of double photoionization of CF4 using time-of-flight photoelectron-photoelectron (photoion-photoion) coincidence spectroscopy. Journal of Chemical Physics, 2006, 125, 194318.	1.2	26
13	The CMS Phase-1 pixel detector upgrade. Journal of Instrumentation, 2021, 16, P02027-P02027.	0.5	25
14	P-Type Silicon Strip Sensors for the new CMS Tracker at HL-LHC. Journal of Instrumentation, 2017, 12, P06018-P06018.	0.5	24
15	BERTHA: Implementation of a four-component Diracâ€“Kohnâ€“Sham relativistic framework. Journal of Chemical Physics, 2020, 152, 164118.	1.2	24
16	Shape and Morphology Effects on the Electronic Structure of TiO₂ Nanostructures: From Nanocrystals to Nanorods. ACS Applied Materials & Interfaces, 2014, 6, 2471-2478.	4.0	22
17	Charge-Displacement Analysis via Natural Orbitals for Chemical Valence in the Four-Component Relativistic Framework. Journal of Chemical Theory and Computation, 2018, 14, 1286-1296.	2.3	22
18	Reactivity of antitumor coinage metal-based N-heterocyclic carbene complexes with cysteine and selenocysteine protein sites. Journal of Inorganic Biochemistry, 2021, 223, 111533.	1.5	22

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19	Efficient Parallel All-Electron Four-Component Diracâ€“Kohnâ€“Sham Program Using a Distributed Matrix Approach II. Journal of Chemical Theory and Computation, 2013, 9, 5356-5364.	2.3	21
20	Full Parallel Implementation of an All-Electron Four-Component Diracâ€“Kohnâ€“Sham Program. Journal of Chemical Theory and Computation, 2014, 10, 3766-3776.	2.3	21
21	Site-selected Auger electron spectroscopy of N2O. Journal of Chemical Physics, 2006, 125, 054306.	1.2	20
22	Predicting protein pK_a by environment similarity. Proteins: Structure, Function and Bioinformatics, 2009, 76, 484-495.	1.5	20
23	Effects of nuclear dynamics in the low-kinetic-energy Auger spectra of CO and CO2. Journal of Chemical Physics, 2005, 123, 224306.	1.2	19
24	Computational investigations of bioinorganic complexes: The case of calcium, gold and platinum ions. AIP Conference Proceedings, 2019, , .	0.3	18
25	Goldâ€“superheavy-element interaction in diatomics and cluster adducts: A combined four-component Dirac-Kohn-Sham/charge-displacement study. Journal of Chemical Physics, 2015, 143, 024307.	1.2	17
26	The Chemical Bond and sâ€“d Hybridization in Coinage Metal(I) Cyanides. Inorganic Chemistry, 2019, 58, 11716-11729.	1.9	17
27	PyBERTHART: A Relativistic Real-Time Four-Component TDDFT Implementation Using Prototyping Techniques Based on Python. Journal of Chemical Theory and Computation, 2020, 16, 2410-2429.	2.3	17
28	Effect of pomegranate peel extract on shelf life of strawberries: computational chemistry approaches to assess antifungal mechanisms involved. Journal of Food Science and Technology, 2018, 55, 2702-2711.	1.4	16
29	Characterization of PD-L1 binding sites by a combined FMO/GRID-DRY approach. Journal of Computer-Aided Molecular Design, 2020, 34, 897-914.	1.3	15
30	Parallelization of a relativistic DFT code. Future Generation Computer Systems, 2004, 20, 739-747.	4.9	14
31	Investigation of the molecular similarity in closely related protein systems: The PrP case study. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1751-1765.	1.5	14
32	An insight of early PrPâ€£200K aggregation by combined molecular dynamics/fragment molecular orbital approaches. Proteins: Structure, Function and Bioinformatics, 2019, 87, 51-61.	1.5	14
33	Spinâ€“orbit coupling is the key to unraveling intriguing features of the halogen bond involving astatine. Physical Chemistry Chemical Physics, 2020, 22, 1897-1910.	1.3	13
34	Environmental Effects with Frozen-Density Embedding in Real-Time Time-Dependent Density Functional Theory Using Localized Basis Functions. Journal of Chemical Theory and Computation, 2020, 16, 5695-5711.	2.3	12
35	Precision measurement of the structure of the CMS inner tracking system using nuclear interactions. Journal of Instrumentation, 2018, 13, P10034-P10034.	0.5	11
36	Implementation and use of a direct, partially integralâ€driven nonâ€Dyson propagator method for molecular ionization. Journal of Computational Chemistry, 2009, 30, 818-825.	1.5	9

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37	The Effects of Ca2+ Concentration and E200K Mutation on the Aggregation Propensity of PrPC: A Computational Study. PLoS ONE, 2016, 11, e0168039.	1.1	9
38	Trapping in proton irradiated p+-n-n+silicon sensors at fluences anticipated at the HL-LHC outer tracker. Journal of Instrumentation, 2016, 11, P04023-P04023.	0.5	8
39	Linear Algebra Computation Benchmarks on a Model Grid Platform. Lecture Notes in Computer Science, 2003, , 297-306.	1.0	8
40	Double photoionization of thiophene and bromine-substituted thiophenes. Journal of Chemical Physics, 2008, 129, 234303.	1.2	7
41	Financial risk distribution in European Union. Physica A: Statistical Mechanics and Its Applications, 2018, 505, 252-267.	1.2	7
42	The Role of APOSTART in Switching between Sexuality and Apomixis in Poa pratensis. Genes, 2020, 11, 941.	1.0	7
43	Impact of low-dose electron irradiation on n+p silicon strip sensors. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2015, 803, 100-112.	0.7	6
44	A database approach for materials selection for hydrogen storage in aerospace technology. Rendiconti Lincei, 2019, 30, 287-296.	1.0	6
45	Beam test performance of prototype silicon detectors for the Outer Tracker for the Phase-2 Upgrade of CMS. Journal of Instrumentation, 2020, 15, P03014-P03014.	0.5	6
46	Combining machine learning and quantum mechanics yields more <scp>chemically aware</scp> molecular descriptors for medicinal chemistry applications. Journal of Computational Chemistry, 2021, 42, 2068-2078.	1.5	6
47	Radiationless decay in the region of the 2t2g and 4eg resonances in SF6. Journal of Chemical Physics, 2011, 134, 094308.	1.2	5
48	Test beam performance measurements for the Phase I upgrade of the CMS pixel detector. Journal of Instrumentation, 2017, 12, P05022-P05022.	0.5	5
49	Experimental study of different silicon sensor options for the upgrade of the CMS Outer Tracker. Journal of Instrumentation, 2020, 15, P04017-P04017.	0.5	5
50	A photoelectron and double photoionization study of the valence electronic structure of 1,4-bromofluorobenzene. Journal of Chemical Physics, 2009, 131, 184302.	1.2	4
51	Modeling Mesoporous Nanoparticulated TiO2Films through Nanopolyhedra Random Packing. Journal of Physical Chemistry C, 2015, 119, 10716-10726.	1.5	4
52	Characterisation of irradiated thin silicon sensors for the CMS phase II pixel upgrade. European Physical Journal C, 2017, 77, 1.	1.4	4
53	Test beam demonstration of silicon microstrip modules with transverse momentum discrimination for the future CMS tracking detector. Journal of Instrumentation, 2018, 13, P03003-P03003.	0.5	4
54	Hampering the early aggregation of PrP-E200K protein by charge-based inhibitors: a computational study. Journal of Computer-Aided Molecular Design, 2021, 35, 751-770.	1.3	4

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55	A cloud-based solution for public administrations: The experience of the Regione Marche. , 2014, , .		3
56	Relativistic quantum chemistry involving heavy atoms. Rendiconti Lincei, 2018, 29, 209-217.	1.0	3
57	A Pattern Recognition Mezzanine based on Associative Memory and FPGA technology for Level 1 Track Triggers for the HL-LHC upgrade. Journal of Instrumentation, 2016, 11, C02063-C02063.	0.5	2
58	A Continuous-Time Inequality Measure Applied to Financial Risk: The Case of the European Union. International Journal of Financial Studies, 2018, 6, 62.	1.1	2
59	The DAQ and control system for the CMS Phase-1 pixel detector upgrade. Journal of Instrumentation, 2019, 14, P10017-P10017.	0.5	2
60	Automated Simulation of Gas-Phase Reactions on Distributed and Cloud Computing Infrastructures. Lecture Notes in Computer Science, 2017, , 60-73.	1.0	2
61	BERTHA and PyBERTHA: State of the Art for Full Four-Component Dirac-Kohn-Sham Calculations. Advances in Parallel Computing, 2020, , .	0.3	2
62	Toward machine learning for microscopic mechanisms: A formula search for crystal structure stability based on atomic properties. Journal of Applied Physics, 2022, 131, .	1.1	2
63	A pattern recognition mezzanine based on associative memory and FPGA technology for L1 track triggering at HL-LHC. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2016, 824, 284-286.	0.7	1
64	A Copula-based Markov Reward Approach to the Credit Spread in the European Union. Applied Mathematical Finance, 2019, 26, 359-386.	0.8	1
65	Reinforcement Learning for Smart Caching at the CMS experiment. , 2021, , .		1
66	A Real-Time Demonstrator for Track Reconstruction in the CMS L1 Track-Trigger System Based on Custom Associative Memories and High-Performance FPGAs. , 2018, , .		1
67	The BondMachine, a moldable computer architecture. Parallel Computing, 2022, 109, 102873.	1.3	1
68	Multitechnique investigation of the valence and inner shell excitation, ionization and decay of halogenated pyrimidines. Journal of Physics: Conference Series, 2009, 194, 022057.	0.3	0
69	Track finding mezzanine for Level-1 triggering in HL-LHC experiments. , 2017, , .		0
70	Mechanical stability of the CMS strip tracker measured with a laser alignment system. Journal of Instrumentation, 2017, 12, P04023-P04023.	0.5	0
71	A model of the three-dimensional structure of human interferon responsive factor 1 and its modifications upon phosphorylation or phosphorylation-mimicking mutations. Journal of Biomolecular Structure and Dynamics, 2019, 37, 4632-4643.	2.0	0
72	Harvesting dispersed computational resources with Openstack: a Cloud infrastructure for the Computational Science community. , 2018, , .		0

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73	On the Sensitivity of a Dynamic Measure of Financial Inequality. Journal of Mathematics and Statistics, 2019, 15, 280-297.	0.2	0
74	The BondMachine toolkit: Enabling Machine Learning on FPGA. , 2019, , .		0
75	Randentropy: A Software to Measure Inequality in Random Systems. Informatica, 2022, , 1-20.	1.5	0