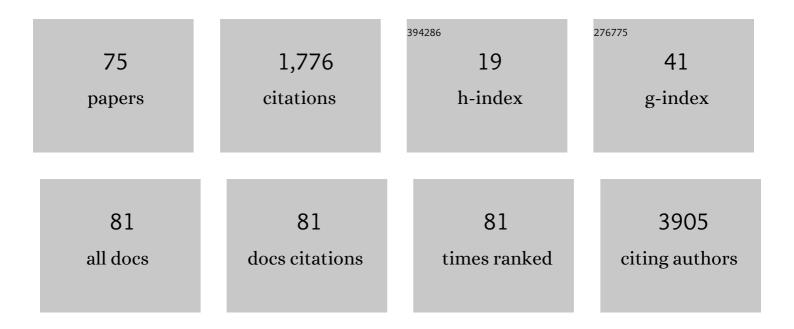
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List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	The BondMachine, a moldable computer architecture. Parallel Computing, 2022, 109, 102873.	1.3	1
2	Randentropy: A Software to Measure Inequality in Random Systems. Informatica, 2022, , 1-20.	1.5	0
3	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
4	The CMS Phase-1 pixel detector upgrade. Journal of Instrumentation, 2021, 16, P02027-P02027.	0.5	25
5	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
6	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
7	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
8	Reinforcement Learning for Smart Caching at the CMS experiment. , 2021, , .		1
9	Spin–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
10	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
11	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
12	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
13	The Role of APOSTART in Switching between Sexuality and Apomixis in Poa pratensis. Genes, 2020, 11, 941.	1.0	7
14	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
15	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
16	BERTHA: Implementation of a four-component Dirac–Kohn–Sham relativistic framework. Journal of Chemical Physics, 2020, 152, 164118.	1.2	24
17	BERTHA and PyBERTHA: State of the Art for Full Four-Component Dirac-Kohn-Sham Calculations. Advances in Parallel Computing, 2020, , .	0.3	2
18	The Chemical Bond and s–d Hybridization in Coinage Metal(I) Cyanides. Inorganic Chemistry, 2019, 58, 11716-11729.	1.9	17

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19	A database approach for materials selection for hydrogen storage in aerospace technology. Rendiconti Lincei, 2019, 30, 287-296.	1.0	6
20	The DAQ and control system for the CMS Phase-1 pixel detector upgrade. Journal of Instrumentation, 2019, 14, P10017-P10017.	0.5	2
21	Computational investigations of bioinorganic complexes: The case of calcium, gold and platinum ions. AIP Conference Proceedings, 2019, , .	0.3	18
22	A Copula-based Markov Reward Approach to the Credit Spread in the European Union. Applied Mathematical Finance, 2019, 26, 359-386.	0.8	1
23	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	Ο
24	An insight of early PrPâ€E200K aggregation by combined molecular dynamics/fragment molecular orbital approaches. Proteins: Structure, Function and Bioinformatics, 2019, 87, 51-61.	1.5	14
25	On the Sensitivity of a Dynamic Measure of Financial Inequality. Journal of Mathematics and Statistics, 2019, 15, 280-297.	0.2	Ο
26	The BondMachine toolkit: Enabling Machine Learning on FPGA. , 2019, , .		0
27	Financial risk distribution in European Union. Physica A: Statistical Mechanics and Its Applications, 2018, 505, 252-267.	1.2	7
28	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
29	Relativistic quantum chemistry involving heavy atoms. Rendiconti Lincei, 2018, 29, 209-217.	1.0	3
30	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
31	Precision measurement of the structure of the CMS inner tracking system using nuclear interactions. Journal of Instrumentation, 2018, 13, P10034-P10034.	0.5	11
32	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
33	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
34	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
35	Harvesting dispersed computational resources with Openstack: a Cloud infrastructure for the Computational Science community. , 2018, , .		0
36	Track finding mezzanine for Level-1 triggering in HL-LHC experiments. , 2017, , .		0

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37	P-Type Silicon Strip Sensors for the new CMS Tracker at HL-LHC. Journal of Instrumentation, 2017, 12, P06018-P06018.	0.5	24
38	Mechanical stability of the CMS strip tracker measured with a laser alignment system. Journal of Instrumentation, 2017, 12, P04023-P04023.	0.5	0
39	Test beam performance measurements for the Phase I upgrade of the CMS pixel detector. Journal of Instrumentation, 2017, 12, P05022-P05022.	0.5	5
40	Characterisation of irradiated thin silicon sensors for the CMS phase II pixel upgrade. European Physical Journal C, 2017, 77, 1.	1.4	4
41	Automated Simulation of Gas-Phase Reactions on Distributed and Cloud Computing Infrastructures. Lecture Notes in Computer Science, 2017, , 60-73.	1.0	2
42	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
43	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
44	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
45	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
46	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
47	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
48	Modeling Mesoporous Nanoparticulated TiO2Films through Nanopolyhedra Random Packing. Journal of Physical Chemistry C, 2015, 119, 10716-10726.	1.5	4
49	Gold–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
50	A cloud-based solution for public administrations: The experience of the Regione Marche. , 2014, , .		3
51	Full Parallel Implementation of an All-Electron Four-Component Dirac–Kohn–Sham Program. Journal of Chemical Theory and Computation, 2014, 10, 3766-3776.	2.3	21
52	Shape and Morphology Effects on the Electronic Structure of TiO ₂ Nanostructures: From Nanocrystals to Nanorods. ACS Applied Materials & Interfaces, 2014, 6, 2471-2478.	4.0	22
53	Inherent electronic trap states in TiO2 nanocrystals: effect of saturation and sintering. Energy and Environmental Science, 2013, 6, 1221.	15.6	76
54	Efficient Parallel All-Electron Four-Component Dirac–Kohn–Sham Program Using a Distributed Matrix Approach II. Journal of Chemical Theory and Computation, 2013, 9, 5356-5364.	2.3	21

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55	Scientific objectives of Einstein Telescope. Classical and Quantum Gravity, 2012, 29, 124013.	1.5	355
56	Recent advances and perspectives in four-component Dirac–Kohn–Sham calculations. Physical Chemistry Chemical Physics, 2011, 13, 12368.	1.3	59
57	Radiationless decay in the region of the 2t2g and 4eg resonances in SF6. Journal of Chemical Physics, 2011, 134, 094308.	1.2	5
58	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
59	An Efficient Parallel All-Electron Four-Component Diracâ	2.3	27
60	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
61	Molecular photoionization cross sections by Stieltjes–Chebyshev moment theory applied to Lanczos pseudospectra. Journal of Chemical Physics, 2009, 130, 064104.	1.2	37
62	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
63	<i>In silico</i> p <i>K</i> _a Prediction and ADME Profiling. Chemistry and Biodiversity, 2009, 6, 1812-1821.	1.0	70
64	Predicting protein p <i>K</i> _a by environment similarity. Proteins: Structure, Function and Bioinformatics, 2009, 76, 484-495.	1.5	20
65	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
66	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
67	The Auger spectroscopy of pyrimidine and halogen-substituted pyrimidines. Journal of Chemical Physics, 2008, 129, 154309.	1.2	28
68	Double photoionization of thiophene and bromine-substituted thiophenes. Journal of Chemical Physics, 2008, 129, 234303.	1.2	7
69	New and Original p <i>K</i> _a Prediction Method Using Grid Molecular Interaction Fields. Journal of Chemical Information and Modeling, 2007, 47, 2172-2181.	2.5	277
70	Site-selected Auger electron spectroscopy of N2O. Journal of Chemical Physics, 2006, 125, 054306.	1.2	20
71	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
72	Complete valence double photoionization of SF6. Journal of Chemical Physics, 2005, 122, 144309.	1.2	29

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73	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
74	Parallelization of a relativistic DFT code. Future Generation Computer Systems, 2004, 20, 739-747.	4.9	14
75	Linear Algebra Computation Benchmarks on a Model Grid Platform. Lecture Notes in Computer Science, 2003, , 297-306.	1.0	8