Carlos H Borca

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7508161/publications.pdf

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23	648	687363 13	677142 22
papers	citations	h-index	g-index

24	24	24	1036
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Octopus, a computational framework for exploring light-driven phenomena and quantum dynamics in extended and finite systems. Journal of Chemical Physics, 2020, 152, 124119.	3.0	210
2	The acid-catalyzed hydrolysis of an <i>Î±</i>-pinene-derived organic nitrate: kinetics, products, reaction mechanisms, and atmospheric impact. Atmospheric Chemistry and Physics, 2016, 16, 15425-15432.	4.9	56
3	Machine Learning on a Robotic Platform for the Design of Polymerâ€“Protein Hybrids. Advanced Materials, 2022, 34, e2201809.	21.0	48
4	A Comparison of the Crystallization Inhibition Properties of Bile Salts. Crystal Growth and Design, 2016, 16, 7286-7300.	3.0	45
5	Mechanistic Design of Chemically Diverse Polymers with Applications in Oral Drug Delivery. Biomacromolecules, 2016, 17, 3659-3671.	5.4	44
6	Featurization strategies for polymer sequence or composition design by machine learning. Molecular Systems Design and Engineering, 2022, 7, 661-676.	3.4	43
7	Photochemical degradation of isoprene-derived 4,1-nitrooxy enal. Atmospheric Chemistry and Physics, 2016, 16, 5595-5610.	4.9	31
8	Machineâ€Assisted Discovery of Chondroitinase ABC Complexes toward Sustained Neural Regeneration. Advanced Healthcare Materials, 2022, 11, e2102101.	7.6	25
9	Crystallization Inhibition Properties of Cellulose Esters and Ethers for a Group of Chemically Diverse Drugs: Experimental and Computational Insight. Biomacromolecules, 2018, 19, 4593-4606.	5.4	20
10	Phase Behavior of Drug-Hydroxypropyl Methylcellulose Amorphous Solid Dispersions Produced from Various Solvent Systems: Mechanistic Understanding of the Role of Polymer using Experimental and Theoretical Methods. Molecular Pharmaceutics, 2018, 15, 3236-3251.	4.6	17
11	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE‹scp›ngine‹/scp›): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801.	3.0	15
12	CrystaLattE: Automated computation of lattice energies of organic crystals exploiting the many-body expansion to achieve dual-level parallelism. Journal of Chemical Physics, 2019, 151, 144103.	3.0	14
13	Connection between Hybrid Functionals and Importance of the Local Density Approximation. Journal of Physical Chemistry A, 2016, 120, 1605-1612.	2.5	13
14	X-ray Fiber Diffraction and Computational Analyses of Stacked Hexads in Supramolecular Polymers: Insight into Self-Assembly in Water by Prospective Prebiotic Nucleobases. Journal of the American Chemical Society, 2021, 143, 6079-6094.	13.7	13
15	Molecular Dynamics of a Water-Absorbent Nanoscale Material Based on Chitosan. Journal of Physical Chemistry B, 2016, 120, 3754-3764.	2.6	11
16	Ground-State Charge Transfer: Lithiumâ€“Benzene and the Role of Hartreeâ€“Fock Exchange. Journal of Physical Chemistry A, 2016, 120, 8190-8198.	2.5	11
17	Domain Separation in Density Functional Theory. Journal of Physical Chemistry A, 2019, 123, 4785-4795.	2.5	10
18	Interaction of Polymers with Enzalutamide Nanodropletsâ€”Impact on Droplet Properties and Induction Times. Molecular Pharmaceutics, 2021, 18, 836-849.	4.6	9

#	Article	IF	Citations
19	Optimization of the synthesis of quinoline-based neutral cyclometalated iridium complexes via microwave irradiation: design of light harvesting and emitting complexes using bulky quinolines. Organic Chemistry Frontiers, 2019, 6, 3374-3382.	4.5	5
20	Morphology of Organic Semiconductors Electrically Doped from Solution Using Phosphomolybdic Acid. Chemistry of Materials, 2019, 31, 6677-6683.	6.7	4
21	To Be or Not To Be Symmetric: That Is the Question for Potentially Active Vibronic Modes. Journal of Chemical Education, 2017, 94, 1232-1237.	2.3	2
22	Machineâ€Assisted Discovery of Chondroitinase ABC Complexes toward Sustained Neural Regeneration (Adv. Healthcare Mater. 10/2022). Advanced Healthcare Materials, 2022, 11, .	7.6	1
23	Domain Separated Density Functional Theory for Reaction Energy Barriers and Optical Excitations. Journal of Physical Chemistry A, 2020, 124, 5954-5962.	2.5	0