Carlos H Borca

List of Publications by Year
in descending order

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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	Machineâ€Assisted Discovery of Chondroitinase ABC Complexes toward Sustained Neural Regeneration. Advanced Healthcare Materials, 2022, 11, e2102101.	7.6	25
2	Featurization strategies for polymer sequence or composition design by machine learning. Molecular Systems Design and Engineering, 2022, 7, 661-676.	3.4	43
3	Machine Learning on a Robotic Platform for the Design of Polymerâ€“Protein Hybrids. Advanced Materials, 2022, 34, e2201809.	21.0	48
4	Machineâ€Assisted Discovery of Chondroitinase ABC Complexes toward Sustained Neural Regeneration (Adv. Healthcare Mater. 10/2022). Advanced Healthcare Materials, 2022, 11, .	7.6	1
5	Interaction of Polymers with Enzalutamide Nanodropletsâ€”Impact on Droplet Properties and Induction Times. Molecular Pharmaceutics, 2021, 18, 836-849.	4.6	9
6	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
7	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
8	Domain Separated Density Functional Theory for Reaction Energy Barriers and Optical Excitations. Journal of Physical Chemistry A, 2020, 124, 5954-5962.	2.5	0
9	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
10	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
11	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
12	Morphology of Organic Semiconductors Electrically Doped from Solution Using Phosphomolybdic Acid. Chemistry of Materials, 2019, 31, 6677-6683.	6.7	4
13	Domain Separation in Density Functional Theory. Journal of Physical Chemistry A, 2019, 123, 4785-4795.	2.5	10
14	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
15	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
16	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
17	Molecular Dynamics of a Water-Absorbent Nanoscale Material Based on Chitosan. Journal of Physical Chemistry B, 2016, 120, 3754-3764.	2.6	11
18	Mechanistic Design of Chemically Diverse Polymers with Applications in Oral Drug Delivery. Biomacromolecules, 2016, 17, 3659-3671.	5.4	44

#	Article	IF	Citations
19	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
20	A Comparison of the Crystallization Inhibition Properties of Bile Salts. Crystal Growth and Design, 2016, 16, 7286-7300.	3.0	45
21	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
22	Photochemical degradation of isoprene-derived 4,1-nitrooxy enal. Atmospheric Chemistry and Physics, 2016, 16, 5595-5610.	4.9	31
23	Connection between Hybrid Functionals and Importance of the Local Density Approximation. Journal of Physical Chemistry A, 2016, 120, 1605-1612.	2.5	13