Brendaâ€M Rubenstein

List of Publications by Year
in descending order

41 papers	931 citations	566801 15 h-index	454577 30 g-index
44 all docs	44 docs citations	44 times ranked	1389 citing authors

#	Article	IF	Citations
1	<tt>QMCPACK</tt>: an open sourceab initioquantum Monte Carlo package for the electronic structure of atoms, molecules and solids. Journal of Physics Condensed Matter, 2018, 30, 195901.	0.7	187
2	The Role of Extracellular Matrix in Glioma Invasion: A Cellular Potts Model Approach. Biophysical Journal, 2008, 95, 5661-5680.	0.2	104
3	Synthesis of All-Inorganic Cd-Doped CsPbCl₃ Perovskite Nanocrystals with Dual-Wavelength Emission. Journal of Physical Chemistry Letters, 2018, 9, 7079-7084.	2.1	92
4	QMCPACK: Advances in the development, efficiency, and application of auxiliary field and real-space variational and diffusion quantum Monte Carlo. Journal of Chemical Physics, 2020, 152, 174105.	1.2	80
5	Pressure-Induced Phase Transformation and Band-Gap Engineering of Formamidinium Lead Iodide Perovskite Nanocrystals. Journal of Physical Chemistry Letters, 2018, 9, 4199-4205.	2.1	78
6	Multicomponent molecular memory. Nature Communications, 2020, 11, 691.	5.8	40
7	Ab InitioFinite Temperature Auxiliary Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2018, 14, 4722-4732.	2.3	39
8	Predicting the viability of beta-lactamase: How folding and binding free energies correlate with beta-lactamase fitness. PLoS ONE, 2020, 15, e0233509.	1.1	26
9	Finite-temperature auxiliary-field quantum Monte Carlo technique for Bose-Fermi mixtures. Physical Review A, 2012, 86, .	1.0	25
10	Observation of a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Ï€</mml:mi></mml:math> -Type Dipole-Bound State in Molecular Anions. Physical Review Letters, 2020, 125, 073003.	2.9	25
11	Accurate Predictions of Electron Binding Energies of Dipole-Bound Anions via Quantum Monte Carlo Methods. Journal of Physical Chemistry Letters, 2018, 9, 6185-6190.	2.1	24
12	Encoding information in synthetic metabolomes. PLoS ONE, 2019, 14, e0217364.	1.1	18
13	A combined first principles study of the structural, magnetic, and phonon properties of monolayer CrI3. Journal of Chemical Physics, 2022, 156, 014707.	1.2	18
14	Principles of Information Storage in Small-Molecule Mixtures. IEEE Transactions on Nanobioscience, 2020, 19, 378-384.	2.2	17
15	Finite temperature auxiliary field quantum Monte Carlo in the canonical ensemble. Journal of Chemical Physics, 2020, 153, 204108.	1.2	17
16	Polarization of Valence Orbitals by the Intramolecular Electric Field from a Diffuse Dipole-Bound Electron. Journal of Physical Chemistry Letters, 2020, 11, 7914-7919.	2.1	15
17	Controlling the Folding and Substrate-Binding of Proteins Using Polymer Brushes. Physical Review Letters, 2012, 108, 208104.	2.9	14
18	Unveiling the Finite Temperature Physics of Hydrogen Chains via Auxiliary Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2020, 16, 4298-4314.	2.3	14

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19	Observation of a Symmetry-Forbidden Excited Quadrupole-Bound State. Journal of the American Chemical Society, 2020, 142, 20240-20246.	6.6	11
20	Maximizing Thermoelectric Figures of Merit by Uniaxially Straining Indium Selenide. Journal of Physical Chemistry C, 2019, 123, 25437-25447.	1.5	9
21	Metal-insulator and magnetic phase diagram of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ca</mml:mi><mml:mn>2</mml:mn></mml	1.1	9
22	van der Waals-corrected density functional study of electric field noise heating in ion traps caused by electrode surface adsorbates. New Journal of Physics, 2019, 21, 053043.	1.2	8
23	Auxiliary field quantum Monte Carlo for multiband Hubbard models: Controlling the sign and phase problems to capture Hund's physics. Physical Review B, 2019, 99, .	1.1	8
24	Real-time dynamics of strongly correlated fermions using auxiliary field quantum Monte Carlo. Journal of Chemical Physics, 2021, 154, 184103.	1.2	8
25	Parallelized Linear Classification with Volumetric Chemical Perceptrons. , 2018, , .		7
26	Evidence from first-principles calculations for orbital ordering in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>Ba</mml:mi></mml:mrow><mml:mn>2</mml	1.1	7
27	A topological data analytic approach for discovering biophysical signatures in protein dynamics. PLoS Computational Biology, 2022, 18, e1010045.	1.5	7
28	Leveraging autocatalytic reactions for chemical domain image classification. Chemical Science, 2021, 12, 5464-5472.	3.7	4
29	LYRUS: a machine learning model for predicting the pathogenicity of missense variants. Bioinformatics Advances, 2022, 2, vbab045.	0.9	4
30	Finite-Size Error Cancellation in Diffusion Monte Carlo Calculations of Surface Chemistry. Journal of Physical Chemistry A, 2022, 126, 4636-4646.	1.1	4
31	A Language for Molecular Computation. CheM, 2019, 5, 3017-3019.	5.8	3
32	First principles calculations of the electric field gradient tensors of Ba₂NaOsO₆, a Mott insulator with strong spin orbit coupling. Journal of Physics Condensed Matter, 2020, 32, 405802.	0.7	3
33	Computing with Chemicals: Perceptrons Using Mixtures of Small Molecules. , 2018, , .		2
34	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mo>/</mml:mo><mml:mi>ï‰</mml:mi	1.0	2
35	Implementing parallel arithmetic via acetylation and its application to chemical image processing. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2021, 477, .	1.0	1
36	Secret messaging with endogenous chemistry. Scientific Reports, 2021, 11, 13960.	1.6	1

#	Article	IF	Citations
37	Title is missing!. , 2020, 15, e0233509.		0
38	Title is missing!. , 2020, 15, e0233509.		0
39	Title is missing!. , 2020, 15, e0233509.		0
40	Title is missing!. , 2020, 15, e0233509.		0
41	Covalent docking and molecular dynamics simulations reveal the specificity-shifting mutations Ala237Arg and Ala237Lys in TEM beta-lactamase. PLoS Computational Biology, 2022, 18, e1009944.	1.5	0