List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Accelerating the prediction of large carbon clusters via structure search: Evaluation of machine-learning and classical potentials. Carbon, 2022, 191, 255-266.	10.3	11
2	SARS-CoV-2 reactive and neutralizing antibodies discovered by single-cell sequencing of plasma cells and mammalian display. Cell Reports, 2022, 38, 110242.	6.4	13
3	High-Temperature Superconductivity in the Lanthanide Hydrides at Extreme Pressures. Applied Sciences (Switzerland), 2022, 12, 874.	2.5	4
4	Exploring the Effect of the Number of Hydrogen Atoms on the Properties of Lanthanide Hydrides by DMFT. Applied Sciences (Switzerland), 2022, 12, 3498.	2.5	0
5	Computational materials discovery for lanthanide hydrides at high pressure for high temperature superconductivity. Physical Review Research, 2022, 4, .	3.6	2
6	In silico proof of principle of machine learning-based antibody design at unconstrained scale. MAbs, 2022, 14, 2031482.	5.2	40
7	Many-Body Study of Iron(III)-Bound Human Serum Transferrin. Journal of Physical Chemistry Letters, 2022, , 4419-4425.	4.6	0
8	Electronic Structure Correspondence of Singlet-Triplet Scale Separation in Strained Sr2RuO4. Applied Sciences (Switzerland), 2021, 11, 508.	2.5	4
9	A compact vocabulary of paratope-epitope interactions enables predictability of antibody-antigen binding. Cell Reports, 2021, 34, 108856.	6.4	101
10	Optimization of therapeutic antibodies by predicting antigen specificity from antibody sequence via deep learning. Nature Biomedical Engineering, 2021, 5, 600-612.	22.5	156
11	Platypus: an open-access software for integrating lymphocyte single-cell immune repertoires with transcriptomes. NAR Genomics and Bioinformatics, 2021, 3, lqab023.	3.2	27
12	Maximally localized dynamical quantum embedding for solving many-body correlated systems. Nature Computational Science, 2021, 1, 410-420.	8.0	6
13	From Slater to Mott physics by epitaxially engineering electronic correlations in oxide interfaces. Npj Computational Materials, 2021, 7, .	8.7	1
14	Study of disorder in pulsed laser deposited double perovskite oxides by first-principle structure prediction. Npj Computational Materials, 2021, 7, .	8.7	4
15	A Single-Cell Atlas of Lymphocyte Adaptive Immune Repertoires and Transcriptomes Reveals Age-Related Differences in Convalescent COVID-19 Patients. Frontiers in Immunology, 2021, 12, 701085.	4.8	33
16	Ultrafast Electron Dynamics in Magnetic Thin Films. Applied Sciences (Switzerland), 2021, 11, 9753.	2.5	4
17	The immuneML ecosystem for machine learning analysis of adaptive immune receptor repertoires. Nature Machine Intelligence, 2021, 3, 936-944.	16.0	35
18	Data-driven dynamical mean-field theory: An error-correction approach to solve the quantum many-body problem using machine learning. Physical Review B. 2021, 104, .	3.2	7

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19	Unifying guiding principles for designing optimized superconductors. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	3
20	Individualized VDJ recombination predisposes the available Ig sequence space. Genome Research, 2021, 31, 2209-2224.	5.5	22
21	Calculating dynamical mean-field theory forces in <i>ab initio</i> ultrasoft pseudopotential formalism. Physical Review B, 2021, 104, .	3.2	6
22	Structural and electronic evolution in the Cu ₃ SbS ₄ –Cu ₃ SnS ₄ solid solution. Journal of Materials Chemistry C, 2020, 8, 11508-11516.	5.5	16
23	ONETEP + TOSCAM: Uniting Dynamical Mean Field Theory and Linear-Scaling Density Functional Theory. Journal of Chemical Theory and Computation, 2020, 16, 4899-4911.	5.3	5
24	immuneSIM: tunable multi-feature simulation of B- and T-cell receptor repertoires for immunoinformatics benchmarking. Bioinformatics, 2020, 36, 3594-3596.	4.1	48
25	Electron–phonon-driven three-dimensional metallicity in an insulating cuprate. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 6409-6416.	7.1	18
26	Superexchange mechanism and quantum many body excitations in the archetypal di-Cu oxo-bridge. Communications Physics, 2020, 3, .	5.3	8
27	Role of the lattice in the light-induced insulator-to-metal transition in vanadium dioxide. Physical Review Research, 2020, 2, .	3.6	9
28	First-principles study of electronic transport and structural properties of Cu12Sb4S13 in its high-temperature phase. Physical Review Research, 2020, 2, .	3.6	10
29	Continuous-time quantum Monte Carlo solver for dynamical mean field theory in the compact Legendre representation. Physical Review B, 2019, 99, .	3.2	9
30	Emergence of long-range magnetic order stabilized by magnetic impurities in pnictides. Physical Review B, 2019, 99, .	3.2	0
31	Tuning topological surface states by cleavage angle in topological crystalline insulators. Physical Review B, 2019, 100, .	3.2	4
32	The Mott to Kondo transition in diluted Kondo superlattices. Communications Physics, 2019, 2, .	5.3	11
33	Evening out the spin and charge parity to increase \$\${T}_{c}\$\$ in \$\${{m{Sr}}}_{2}{{m{RuO}}}_{4}\$\$. Communications Physics, 2019, 2, .	5.3	26
34	Nanoscopic time crystal obtained by nonergodic spin dynamics. Physical Review B, 2019, 100, .	3.2	4
35	Enhanced thermoelectric performance of Sn-doped Cu ₃ SbS ₄ . Journal of Materials Chemistry C, 2018, 6, 8546-8552.	5.5	59
36	Computational Strategies for Dissecting the High-Dimensional Complexity of Adaptive Immune Repertoires. Frontiers in Immunology, 2018, 9, 224.	4.8	164

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37	Metal-Insulator Transition in Copper Oxides Induced by Apex Displacements. Physical Review X, 2018, 8, .	8.9	11
38	Many-body renormalization of forces in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>f</mml:mi> -electron materials. Physical Review B, 2018, 98, .</mml:math 	3.2	20
39	High-throughput antibody engineering in mammalian cells by CRISPR/Cas9-mediated homology-directed mutagenesis. Nucleic Acids Research, 2018, 46, 7436-7449.	14.5	61
40	Systems Analysis Reveals High Genetic and Antigen-Driven Predetermination of Antibody Repertoires throughout B Cell Development. Cell Reports, 2017, 19, 1467-1478.	6.4	172
41	What controls the critical temperature of high temperature copper oxide superconductors: insights from scanneling tunnelling microscopy. Science Bulletin, 2017, 62, 102-104.	9.0	4
42	Learning the High-Dimensional Immunogenomic Features That Predict Public and Private Antibody Repertoires. Journal of Immunology, 2017, 199, 2985-2997.	0.8	124
43	Self-energies in itinerant magnets: A focus on Fe and Ni. Physical Review B, 2017, 95, .	3.2	39
44	Theory-Guided Synthesis of an Eco-Friendly and Low-Cost Copper Based Sulfide Thermoelectric Material. Journal of Physical Chemistry C, 2016, 120, 27135-27140.	3.1	60
45	Renormalization of myoglobin–ligand binding energetics by quantum many-body effects. Proceedings of the United States of America, 2014, 111, 5790-5795.	7.1	33
46	Phase Diagram of a Three-Orbital Model for High- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>T</mml:mi></mml:mrow><mml:mrow><mm Superconductors. Physical Review Letters, 2014, 112, 117001.</mm </mml:mrow></mml:msub></mml:mrow></mml:math 	ıl:mi ^{7.8} <td>ml:mi></td>	ml:mi>
47	Importance of Many-Body Effects in the Kernel of Hemoglobin for Ligand Binding. Physical Review Letters, 2013, 110, 106402.	7.8	29
48	Impurity model for non-equilibrium steady states. Physical Review B, 2013, 87, .	3.2	11
49	Sedimentation of macroscopic rigid knots and its relation to gel electrophoretic mobility of DNA knots. Scientific Reports, 2013, 3, 1091.	3.3	14
50	Scaling of the transition temperature of hole-doped cuprate superconductors with the charge-transfer energy. Europhysics Letters, 2012, 100, 37001.	2.0	85
51	Anticollinear magnetic order induced by impurities in the frustrated Heisenberg model of pnictides. Physical Review B, 2012, 86, .	3.2	11
52	Approach to a stationary state in a driven Hubbard model coupled to a thermostat. Physical Review B, 2012, 86, .	3.2	56
53	Dimensional Crossover Driven by an Electric Field. Physical Review Letters, 2012, 108, 086401.	7.8	52
54	Vanadium Dioxide: A Peierls-Mott Insulator Stable against Disorder. Physical Review Letters, 2012, 108, 256402.	7.8	156

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55	Augmented hybrid exact-diagonalization solver for dynamical mean field theory. Physical Review B, 2012, 86, .	3.2	23
56	High-frequency thermoelectric response in correlated electronic systems. Physical Review B, 2011, 84, .	3.2	10
57	Strength of correlations in electron- and hole-doped cuprates. Nature Physics, 2010, 6, 574-578.	16.7	142
58	Apical oxygens and correlation strength in electron- and hole-doped copper oxides. Physical Review B, 2010, 82, .	3.2	90
59	Orbital Currents in Extended Hubbard Models of High- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>T</mml:mi><mml:mi>c</mml:mi></mml:msub>Cuprate Superconductors, Physical Raview Letters, 2009, 102, 017005.</mml:math 	7.8	99
60	Optical weights and waterfails in doped charge-transfer insulators: A local density approximation and dynamical mean-field theory study of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>La</mml:mtext></mml:mrow><mml:mrow> Physical Population B 2008 78</mml:mrow></mml:msub></mml:mrow></mml:math 	3.2 > < mml:mr	62 1>2
61	Local selection rules that can determine specific pathways of DNA unknotting by type II DNA topoisomerases. Nucleic Acids Research, 2007, 35, 5223-5231.	14.5	39
62	Checkerboard order in the $\hat{a} \in $ model on the square lattice. Journal of Magnetism and Magnetic Materials, 2007, 310, 523-525.	2.3	2
63	Numerical Simulation of Gel Electrophoresis of DNA Knots in Weak and Strong Electric Fields. Biophysical Journal, 2006, 90, 3100-3105.	0.5	37
64	Bond-order-modulated staggered-flux phase of thetJmodel on a square lattice. Physical Review B, 2006, 74, .	3.2	10
65	Simulations of electrophoretic collisions of DNA knots with gel obstacles. Journal of Physics Condensed Matter, 2006, 18, S161-S171.	1.8	11
66	Magnetism and superconductivity of strongly correlated electrons on the triangular lattice. Physical Review B, 2006, 73, .	3.2	42
67	Finite-temperature properties of frustrated classical spins coupled to the lattice. Physical Review B, 2005, 72, .	3.2	22
68	Scanning-Tunneling Spectroscopy of Surface-State Electrons Scattered by a Slightly Disordered Two-Dimensional Dilute "Solid― Ce on Ag(111). Physical Review Letters, 2004, 93, 146805.	7.8	40
69	Ising Transition Driven by Frustration in a 2D Classical Model with Continuous Symmetry. Physical Review Letters, 2003, 91, 177202.	7.8	87