James R Chelikowsky

List of Publications by Year
in descending order

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60 papers	4,623 citations	279701 23 h-index	138417 58 g-index
62 all docs	62 docs citations	62 times ranked	3086 citing authors

#	Article	IF	Citations
1	Predicting magnetic anisotropy energies using site-specific spin-orbit coupling energies and machine learning: Application to iron-cobalt nitrides. Physical Review Materials, 2022, 6, .	0.9	3
2	Quasiparticle energies and optical excitations of 3C-SiC divacancy from <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:n and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:n plus Bethe-Salpeter equationÂcalculations. Physical Review Materials, 2022, 6, .	0.9	6
3	Role of carbon in modifying the properties of superconducting hydrogen sulfide. Physical Review Materials, 2022, 6, .	0.9	0
4	Dielectric screening and vacancy formation for large neutral and charged <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>Si</mml:mi></mml:mrow><mml:mi>n</mml mathvariant="normal">H</mml:mi></mml:mrow><mml:mi>m</mml:mi></mml:msub></mml:math> <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>(</mml:mo><mml:mi>n</mml:mi><mml:mo>></mml: na. Physical Review Materials, 2022, 6, .	0.9	2
5	Space-Filling Curves for Real-Space Electronic Structure Calculations. Journal of Chemical Theory and Computation, 2021, 17, 4039-4048.	2.3	11
6	Atomic Fingerprinting of Heteroatoms Using Noncontact Atomic Force Microscopy. Small, 2021, , 2102977.	5.2	3
7	Breaking a dative bond with mechanical forces. Nature Communications, 2021, 12, 5635.	5.8	17
8	Prediction of Intrinsic Ferroelectricity and Large Piezoelectricity in Monolayer Arsenic Chalcogenides. Nano Letters, 2020, 20, 8346-8352.	4.5	28
9	Synergistic computational and experimental discovery of novel magnetic materials. Molecular Systems Design and Engineering, 2020, 5, 1098-1117.	1.7	13
10	Scalable implementation of polynomial filtering for density functional theory calculation in PARSEC. Computer Physics Communications, 2020, 254, 107330.	3.0	12
11	Accelerating Time-Dependent Density Functional Theory and GW Calculations for Molecules and Nanoclusters with Symmetry Adapted Interpolative Separable Density Fitting. Journal of Chemical Theory and Computation, 2020, 16, 2216-2223.	2.3	19
12	Chemical and steric effects in simulating noncontact atomic force microscopy images of organic molecules on a Cu (111) substrate. Physical Review Materials, 2020, 4, .	0.9	6
13	Discovering rare-earth-free magnetic materials through the development of a database. Physical Review Materials, 2020, 4, .	0.9	11
14	Metastable B-doped FeNi compounds for permanent magnets without rare earths. Physical Review Materials, 2020, 4, .	0.9	1
15	Discrimination of Bond Order in Organic Molecules Using Noncontact Atomic Force Microscopy. Nano Letters, 2019, 19, 5562-5567.	4.5	11
16	Optically Driven Magnetic Phase Transition of Monolayer RuCl₃. Nano Letters, 2019, 19, 7673-7680.	4.5	45
17	Real-Space Based Benchmark of G₀W₀ Calculations on GW100: Effects of Semicore Orbitals and Orbital Reordering. Journal of Chemical Theory and Computation, 2019, 15, 5299-5307.	2.3	13
18	Enhanced magnetic moments in Mn-doped FeCo clusters owing to ferromagnetic surface Mn atoms. Physical Review Materials, 2019, 3, .	0.9	5

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19	Simulating noncontact atomic force microscopy images. Physical Review Materials, 2019, 3, .	0.9	7
20	Simulating the effect of boron doping in superconducting carbon. Physical Review B, 2018, 97, .	1.1	17
21	Real-space pseudopotential calculations for simulating noncontact atomic force microscopy images. Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics, 2018, 36, .	0.6	5
22	The stability, electronic structure, and optical absorption of boron-nitride diamondoids predicted with first-principles calculations. Physical Chemistry Chemical Physics, 2018, 20, 19188-19194.	1.3	5
23	Influence of nitrogen dopants on the magnetization of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Co</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math> clusters. Physical Review Materials,	0.9	7
24	Magnetocrystalline anisotropy in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>YCo</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ZrCo</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:math> compounds from first-principles real-space pseudopotentials calculations. Physical Review Materials, 2018, 2, .	0.9	4
25	Real-space pseudopotential method for calculating magnetocrystalline anisotropy. Physical Review Materials, 2018, 2, .	0.9	7
26	Simulating contrast inversion in atomic force microscopy imaging with real-space pseudopotentials. Physical Review B, 2017, 95, .	1.1	9
27	Formation enthalpies for transition metal alloys using machine learning. Physical Review B, 2017, 95, .	1.1	24
28	First-Principles Atomic Force Microscopy Image Simulations with Density Embedding Theory. Nano Letters, 2016, 16, 3242-3246.	4.5	23
29	Excitation spectra of aromatic molecules within a real-space<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math> formalism: Role of self-consistency and vertex corrections. Physical Review B, 2016, 94, .	1.1	58
30	Size dependence of structural stability and magnetization of nickel clusters from real-space pseudopotentials. Physical Review B, 2016, 94, .	1.1	7
31	Structural and magnetic properties of large cobalt clusters. Physical Review B, 2016, 93, .	1.1	18
32	Repulsive tip tilting as the dominant mechanism for hydrogen bond-like features in atomic force microscopy imaging. Applied Physics Letters, 2016, 108, 193102.	1.5	17
33	CO tip functionalization in subatomic resolution atomic force microscopy. Applied Physics Letters, 2015, 107, .	1.5	18
34	An effective capacitance model for computing the electronic properties of charged defects in crystals. Computer Physics Communications, 2014, 185, 1564-1569.	3.0	4
35	Chebyshev-filtered subspace iteration method free of sparse diagonalization for solving the Kohnâ€“Sham equation. Journal of Computational Physics, 2014, 274, 770-782.	1.9	57
36	Simulated non-contact atomic force microscopy for GaAs surfaces based on real-space pseudopotentials. Applied Surface Science, 2014, 303, 163-167.	3.1	11

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37	Data mining for materials: Computational experiments with<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>A</mml:mi><mml:mi>B</mml:mi></mml:mrow></mml:math>compounds. Physical Review B, 2012, 85, .	1.1	90
38	A spectrum slicing method for the Kohnâ€“Sham problem. Computer Physics Communications, 2012, 183, 497-505.	3.0	98
39	Vacancies and B doping in Si nanocrystals. Solid State Communications, 2010, 150, 130-132.	0.9	15
40	Numerical Methods for Electronic Structure Calculations of Materials. SIAM Review, 2010, 52, 3-54.	4.2	231
41	Efficient First-Principles Simulation of Noncontact Atomic Force Microscopy for Structural Analysis. Physical Review Letters, 2009, 102, 176101.	2.9	18
42	Real-space pseudopotential method for first principles calculations of general periodic and partially periodic systems. Physical Review B, 2008, 78, .	1.1	79
43	Algorithms for the evolution of electronic properties in nanocrystals. Computer Physics Communications, 2007, 177, 1-5.	3.0	8
44	The structure and properties of vacancies in Si nano-crystals calculated by real space pseudopotential methods. Physica B: Condensed Matter, 2007, 401-402, 537-540.	1.3	8
45	Self-Purification in Semiconductor Nanocrystals. Physical Review Letters, 2006, 96, 226802.	2.9	613
46	Evolution of Magnetism in Iron from the Atom to the Bulk. Physical Review Letters, 2006, 97, 147201.	2.9	82
47	Optical excitations in organic molecules, clusters, and defects studied by first-principles Greenâ€™s function methods. Physical Review B, 2006, 73, .	1.1	184
48	PARSEC â€“ the pseudopotential algorithm for real-space electronic structure calculations: recent advances and novel applications to nano-structures. Physica Status Solidi (B): Basic Research, 2006, 243, 1063-1079.	0.7	285
49	Self-consistent-field calculations using Chebyshev-filtered subspace iteration. Journal of Computational Physics, 2006, 219, 172-184.	1.9	152
50	Parallel self-consistent-field calculations via Chebyshev-filtered subspace acceleration. Physical Review E, 2006, 74, 066704.	0.8	145
51	Real-space pseudopotential method for computing the electronic properties of periodic systems. Physical Review B, 2004, 69, .	1.1	83
52	Ab InitioCalculations for Large Dielectric Matrices of Confined Systems. Physical Review Letters, 2003, 90, 127401.	2.9	66
53	First-principles density-functional calculations for optical spectra of clusters and nanocrystals. Physical Review B, 2002, 65, .	1.1	155
54	Ab initioinvestigation of point defects in bulk Si and Ge using a cluster method. Physical Review B, 2001, 64, .	1.1	47

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55	The pseudopotential-density functional method applied to nanostructures. Journal Physics D: Applied Physics, 2000, 33, R33-R50.	1.3	121
56	Ab initiocluster calculations for vacancies in bulk Si. Physical Review B, 1997, 56, R11353-R11356.	1.1	43
57	Higher-order finite-difference pseudopotential method: An application to diatomic molecules. Physical Review B, 1994, 50, 11355-11364.	1.1	506
58	Finite-difference-pseudopotential method: Electronic structure calculations without a basis. Physical Review Letters, 1994, 72, 1240-1243.	2.9	789
59	Electronic Structure and Optical Properties of Semiconductors. Springer Series in Solid-state Sciences, 1989, , .	0.3	305
60	Numerical methods for efficient GW calculations and the applications in low-dimensional systems. Electronic Structure, 0, , .	1.0	1