

James R Chelikowsky

List of Publications by Year in descending order

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60
papers

4,623
citations

279701

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138417

58
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62
all docs

62
docs citations

62
times ranked

3086
citing authors

#	ARTICLE	IF	CITATIONS
1	Finite-difference-pseudopotential method: Electronic structure calculations without a basis. Physical Review Letters, 1994, 72, 1240-1243.	2.9	789
2	Self-Purification in Semiconductor Nanocrystals. Physical Review Letters, 2006, 96, 226802.	2.9	613
3	Higher-order finite-difference pseudopotential method: An application to diatomic molecules. Physical Review B, 1994, 50, 11355-11364.	1.1	506
4	Electronic Structure and Optical Properties of Semiconductors. Springer Series in Solid-state Sciences, 1989, , .	0.3	305
5	PARSEC – 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
6	Numerical Methods for Electronic Structure Calculations of Materials. SIAM Review, 2010, 52, 3-54.	4.2	231
7	Optical excitations in organic molecules, clusters, and defects studied by first-principles Green's function methods. Physical Review B, 2006, 73, .	1.1	184
8	First-principles density-functional calculations for optical spectra of clusters and nanocrystals. Physical Review B, 2002, 65, .	1.1	155
9	Self-consistent-field calculations using Chebyshev-filtered subspace iteration. Journal of Computational Physics, 2006, 219, 172-184.	1.9	152
10	Parallel self-consistent-field calculations via Chebyshev-filtered subspace acceleration. Physical Review E, 2006, 74, 066704.	0.8	145
11	The pseudopotential-density functional method applied to nanostructures. Journal Physics D: Applied Physics, 2000, 33, R33-R50.	1.3	121
12	A spectrum slicing method for the Kohn-Sham problem. Computer Physics Communications, 2012, 183, 497-505.	3.0	98
13	Data mining for materials: Computational experiments with $\langle A \rangle_B$ compounds. Physical Review B, 2012, 85, .	1.1	90
14	Real-space pseudopotential method for computing the electronic properties of periodic systems. Physical Review B, 2004, 69, .	1.1	83
15	Evolution of Magnetism in Iron from the Atom to the Bulk. Physical Review Letters, 2006, 97, 147201.	2.9	82
16	Real-space pseudopotential method for first principles calculations of general periodic and partially periodic systems. Physical Review B, 2008, 78, .	1.1	79
17	Ab Initio Calculations for Large Dielectric Matrices of Confined Systems. Physical Review Letters, 2003, 90, 127401.	2.9	66
18	Chebyshev-filtered subspace iteration method free of sparse diagonalization for solving the Kohn-Sham equation. Journal of Computational Physics, 2014, 274, 770-782.	1.9	57

#	ARTICLE	IF	CITATIONS
19	Excitation spectra of aromatic molecules within a real-space G_0W_0 formalism: Role of self-consistency and vertex corrections. Physical Review B, 2016, 94, .	4.1	58
20	Ab initio investigation of point defects in bulk Si and Ge using a cluster method. Physical Review B, 2001, 64, .	1.1	47
21	Optically Driven Magnetic Phase Transition of Monolayer $RuCl_3$. Nano Letters, 2019, 19, 7673-7680.	4.5	45
22	Ab initio cluster calculations for vacancies in bulk Si. Physical Review B, 1997, 56, R11353-R11356.	1.1	43
23	Prediction of Intrinsic Ferroelectricity and Large Piezoelectricity in Monolayer Arsenic Chalcogenides. Nano Letters, 2020, 20, 8346-8352.	4.5	28
24	Formation enthalpies for transition metal alloys using machine learning. Physical Review B, 2017, 95, .	1.1	24
25	First-Principles Atomic Force Microscopy Image Simulations with Density Embedding Theory. Nano Letters, 2016, 16, 3242-3246.	4.5	23
26	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
27	Efficient First-Principles Simulation of Noncontact Atomic Force Microscopy for Structural Analysis. Physical Review Letters, 2009, 102, 176101.	2.9	18
28	CO tip functionalization in subatomic resolution atomic force microscopy. Applied Physics Letters, 2015, 107, .	1.5	18
29	Structural and magnetic properties of large cobalt clusters. Physical Review B, 2016, 93, .	1.1	18
30	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
31	Simulating the effect of boron doping in superconducting carbon. Physical Review B, 2018, 97, .	1.1	17
32	Breaking a dative bond with mechanical forces. Nature Communications, 2021, 12, 5635.	5.8	17
33	Vacancies and B doping in Si nanocrystals. Solid State Communications, 2010, 150, 130-132.	0.9	15
34	Real-Space Based Benchmark of G_0W_0 Calculations on GW100: Effects of Semicore Orbitals and Orbital Reordering. Journal of Chemical Theory and Computation, 2019, 15, 5299-5307.	2.3	13
35	Synergistic computational and experimental discovery of novel magnetic materials. Molecular Systems Design and Engineering, 2020, 5, 1098-1117.	1.7	13
36	Scalable implementation of polynomial filtering for density functional theory calculation in PARSEC. Computer Physics Communications, 2020, 254, 107330.	3.0	12

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37	Simulated non-contact atomic force microscopy for GaAs surfaces based on real-space pseudopotentials. Applied Surface Science, 2014, 303, 163-167.	3.1	11
38	Discrimination of Bond Order in Organic Molecules Using Noncontact Atomic Force Microscopy. Nano Letters, 2019, 19, 5562-5567.	4.5	11
39	Space-Filling Curves for Real-Space Electronic Structure Calculations. Journal of Chemical Theory and Computation, 2021, 17, 4039-4048.	2.3	11
40	Discovering rare-earth-free magnetic materials through the development of a database. Physical Review Materials, 2020, 4, .	0.9	11
41	Simulating contrast inversion in atomic force microscopy imaging with real-space pseudopotentials. Physical Review B, 2017, 95, .	1.1	9
42	Algorithms for the evolution of electronic properties in nanocrystals. Computer Physics Communications, 2007, 177, 1-5.	3.0	8
43	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
44	Size dependence of structural stability and magnetization of nickel clusters from real-space pseudopotentials. Physical Review B, 2016, 94, .	1.1	7
45	Influence of nitrogen dopants on the magnetization of Co_3N clusters. Physical Review Materials, 2018, 2, .	0.9	7
46	Real-space pseudopotential method for calculating magnetocrystalline anisotropy. Physical Review Materials, 2018, 2, .	0.9	7
47	Simulating noncontact atomic force microscopy images. Physical Review Materials, 2019, 3, .	0.9	7
48	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
49	Quasiparticle energies and optical excitations of 3C-SiC divacancy from GW and $\text{GW} + \text{Bethe-Salpeter}$ equation calculations. Physical Review Materials, 2022, 6, .	0.9	6
50	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
51	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
52	Enhanced magnetic moments in Mn-doped FeCo clusters owing to ferromagnetic surface Mn atoms. Physical Review Materials, 2019, 3, .	0.9	5
53	An effective capacitance model for computing the electronic properties of charged defects in crystals. Computer Physics Communications, 2014, 185, 1564-1569.	3.0	4
54	Magnetocrystalline anisotropy in YCo_5 and ZrCo_5 compounds from first-principles real-space pseudopotentials calculations. Physical Review Materials, 2018, 2, .	0.9	4

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55	Atomic Fingerprinting of Heteroatoms Using Noncontact Atomic Force Microscopy. Small, 2021, , 2102977.	5.2	3
56	Predicting magnetic anisotropy energies using site-specific spin-orbit coupling energies and machine learning: Application to iron-cobalt nitrides. Physical Review Materials, 2022, 6, . Dielectric screening and vacancy formation for large neutral and charged $\langle \text{mml:math}$	0.9	3
57	$\langle \text{mml:math}$ $\langle \text{mml:math}$ $\langle \text{mml:math}$ na. Physical Review Materials, 2022, 6.	0.9	2
58	Metastable B-doped FeNi compounds for permanent magnets without rare earths. Physical Review Materials, 2020, 4, .	0.9	1
59	Numerical methods for efficient GW calculations and the applications in low-dimensional systems. Electronic Structure, 0, , .	1.0	1
60	Role of carbon in modifying the properties of superconducting hydrogen sulfide. Physical Review Materials, 2022, 6, .	0.9	0