InÃªs Lima Azevedo

List of Publications by Year
in descending order

193 papers	8,987 citations	61984 43 h-index	46799 89 g-index
199 all docs	199 docs citations	199 times ranked	8797 citing authors

#	Article	IF	Citations
1	Net-zero emissions energy systems. Science, 2018, 360, .	12.6	1,165
2	Finite-difference-pseudopotential method: Electronic structure calculations without a basis. Physical Review Letters, 1994, 72, 1240-1243.	7.8	789
3	Global food system emissions could preclude achieving the 1.5Â° and 2Â°C climate change targets. Science, 2020, 370, 705-708.	12.6	496
4	A review of learning rates for electricity supply technologies. Energy Policy, 2015, 86, 198-218.	8.8	407
5	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.	1.5	285
6	Numerical Methods for Electronic Structure Calculations of Materials. SIAM Review, 2010, 52, 3-54.	9.5	231
7	Negative Poisson ratios in crystalline SiO2 from first-principles calculations. Nature, 1992, 358, 222-224.	27.8	201
8	Optical excitations in organic molecules, clusters, and defects studied by first-principles Greenâ€™s function methods. Physical Review B, 2006, 73, .	3.2	184
9	Surface oxidation effects on the optical properties of silicon nanocrystals. Physical Review B, 2002, 65, .	3.2	175
10	Estimating direct and indirect rebound effects for U.S. households with inputâ€“output analysis Part 1: Theoretical framework. Ecological Economics, 2013, 86, 199-210.	5.7	174
11	Atomically precise graphene nanoribbon heterojunctions from a single molecular precursor. Nature Nanotechnology, 2017, 12, 1077-1082.	31.5	162
12	Benchmark of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>methods for azabenzenes. Physical Review B, 2012, 86, .	3.2	154
13	Self-consistent-field calculations using Chebyshev-filtered subspace iteration. Journal of Computational Physics, 2006, 219, 172-184.	3.8	152
14	Regional Variability and Uncertainty of Electric Vehicle Life Cycle CO₂ Emissions across the United States. Environmental Science & Technology, 2015, 49, 8844-8855.	10.0	147
15	Parallel self-consistent-field calculations via Chebyshev-filtered subspace acceleration. Physical Review E, 2006, 74, 066704.	2.1	145
16	The pseudopotential-density functional method applied to nanostructures. Journal Physics D: Applied Physics, 2000, 33, R33-R50.	2.8	121
17	Expert assessments of the cost and expected future performance of proton exchange membrane fuel cells for vehicles. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 4899-4904.	7.1	118
18	Estimating direct and indirect rebound effects for U.S. households with inputâ€“output analysis. Part 2: Simulation. Ecological Economics, 2013, 86, 188-198.	5.7	114

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19	Consumer End-Use Energy Efficiency and Rebound Effects. Annual Review of Environment and Resources, 2014, 39, 393-418.	13.4	112
20	The impact of federal incentives on the adoption of hybrid electric vehicles in the United States. Energy Economics, 2013, 40, 936-942.	12.1	110
21	Spectroscopic Evidence for the Tricapped Trigonal Prism Structure of Semiconductor Clusters. Physical Review Letters, 2000, 85, 1666-1669.	7.8	91
22	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, .	3.2	90
23	Decarbonizing intraregional freight systems with a focus on modal shift. Environmental Research Letters, 2018, 13, 083001.	5.2	89
24	Electronic structure of copper phthalocyanine from<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:msub><mml:msub><mml:mi>W</mml: Physical Review B, 2011, 84, .	3.2	86
25	Effect of regional grid mix, driving patterns and climate on the comparative carbon footprint of gasoline and plug-in electric vehicles in the United States. Environmental Research Letters, 2016, 11, 044007.	5.2	84
26	Real-space pseudopotential method for computing the electronic properties of periodic systems. Physical Review B, 2004, 69, .	3.2	83
27	Fine Particulate Air Pollution from Electricity Generation in the US: Health Impacts by Race, Income, and Geography. Environmental Science & Technology, 2019, 53, 14010-14019.	10.0	83
28	Bulk Energy Storage Increases United States Electricity System Emissions. Environmental Science & Technology, 2015, 49, 3203-3210.	10.0	82
29	Structural transformation of quartz at high pressures. Nature, 1991, 353, 344-346.	27.8	80
30	Real-space pseudopotential method for first principles calculations of general periodic and partially periodic systems. Physical Review B, 2008, 78, .	3.2	79
31	Comparison of Life Cycle Greenhouse Gases from Natural Gas Pathways for Medium and Heavy-Duty Vehicles. Environmental Science & Technology, 2015, 49, 7123-7133.	10.0	77
32	Evidence of a Reentrant Peierls Distortion in Liquid GeTe. Physical Review Letters, 2000, 85, 1950-1953.	7.8	76
33	Fine particulate matter damages and value added in the US economy. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 19857-19862.	7.1	74
34	Labeling energy cost on light bulbs lowers implicit discount rates. Ecological Economics, 2014, 97, 42-50.	5.7	72
35	Optical properties of CdSe quantum dots. Journal of Chemical Physics, 2003, 119, 2284-2287.	3.0	71
36	Reducing Mortality from Air Pollution in the United States by Targeting Specific Emission Sources. Environmental Science and Technology Letters, 2020, 7, 639-645.	8.7	64

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37	Comparison of Life Cycle Greenhouse Gases from Natural Gas Pathways for Light-Duty Vehicles. Energy & Fuels, 2015, 29, 6008-6018.	5.1	58
38	Ab initiostructures and polarizabilities of sodium clusters. Journal of Chemical Physics, 2001, 115, 4322-4332.	3.0	56
39	Electronic and optical excitations in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ag</mml:mtext></mml:mrow><mml:mi>n</mml:mi></mml:msub xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mi>n</mml:mi><mml:mo>=</mml:mo><mml:mn Physical Review B, 2009, 79, .	3.2	56
40	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:m formalism: Role of self-consistency and vertex corrections. Physical Review B, 2016, 94, .	3.2	53
41	Assessing the evolution of power sector carbon intensity in the United States. Environmental Research Letters, 2018, 13, 064018.	5.2	52
42	Melting of small Sn clusters byab initiomolecular dynamics simulations. Physical Review B, 2004, 69, .	3.2	50
43	Local structure of liquid GeTe via neutron scattering andab initiosimulations. Physical Review B, 2002, 65, .	3.2	47
44	Was it worthwhile? Where have the benefits of rooftop solar photovoltaic generation exceeded the cost?. Environmental Research Letters, 2017, 12, 094015.	5.2	45
45	Electronic structure of dye-sensitized TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>clusters from many-body perturbation theory. Physical Review B, 2011, 84, .	3.2	41
46	Energy Efficiency: What Has Research Delivered in the Last 40 Years?. Annual Review of Environment and Resources, 2021, 46, 135-165.	13.4	41
47	Edison Revisited: Should we use DC circuits for lighting in commercial buildings?. Energy Policy, 2012, 45, 399-411.	8.8	40
48	Consumersâ€™ perceptions of energy use and energy savings: A literature review. Environmental Research Letters, 2018, 13, 033004.	5.2	34
49	Reduced-Order Dispatch Model for Simulating Marginal Emissions Factors for the United States Power Sector. Environmental Science & Technology, 2019, 53, 10506-10513.	10.0	34
50	Cumulative environmental and employment impacts of the shale gas boom. Nature Sustainability, 2019, 2, 1122-1131.	23.7	34
51	Marginal Emissions Factors for Electricity Generation in the Midcontinent ISO. Environmental Science & Technology, 2017, 51, 14445-14452.	10.0	31
52	Do tidal stream energy projects offer more value than offshore wind farms? A case study in the United Kingdom. Energy Policy, 2018, 113, 28-40.	8.8	31
53	Optimizing Emissions Reductions from the U.S. Power Sector for Climate and Health Benefits. Environmental Science & Technology, 2020, 54, 7513-7523.	10.0	31
54	Lessons from wind policy in Portugal. Energy Policy, 2017, 103, 193-202.	8.8	29

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55	Estimation of the year-on-year volatility and the unpredictability of the United States energy system. Nature Energy, 2018, 3, 341-346.	39.5	29
56	Hybrid density functional study of oligothiophene/ZnO interface for photovoltaics. Physical Review B, 2011, 83, .	3.2	28
57	Size Effects in the Interface Level Alignment of Dye-Sensitized TiO₂ Clusters. Journal of Physical Chemistry Letters, 2014, 5, 2395-2401.	4.6	28
58	Prediction of Intrinsic Ferroelectricity and Large Piezoelectricity in Monolayer Arsenic Chalcogenides. Nano Letters, 2020, 20, 8346-8352.	9.1	28
59	Spatially resolved air-water emissions tradeoffs improve regulatory impact analyses for electricity generation. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 1862-1867.	7.1	26
60	Transport properties of transition-metal-encapsulated Si cages. Physical Review B, 2008, 77, .	3.2	25
61	What are the best combinations of fuel-vehicle technologies to mitigate climate change and air pollution effects across the United States?. Environmental Research Letters, 2020, 15, 074046.	5.2	25
62	The impact of Uber and Lyft on vehicle ownership, fuel economy, and transit across U.S. cities. IScience, 2021, 24, 101933.	4.1	25
63	Consistency and robustness of forecasting for emerging technologies: The case of Li-ion batteries for electric vehicles. Energy Policy, 2017, 106, 415-426.	8.8	24
64	Formation enthalpies for transition metal alloys using machine learning. Physical Review B, 2017, 95, .	3.2	24
65	A sunny future: expert elicitation of China's solar photovoltaic technologies. Environmental Research Letters, 2018, 13, 034038.	5.2	24
66	First principles simulations of SiGe for the liquid and amorphous states. Journal of Chemical Physics, 2002, 117, 3476-3483.	3.0	23
67	First-Principles Atomic Force Microscopy Image Simulations with Density Embedding Theory. Nano Letters, 2016, 16, 3242-3246.	9.1	23
68	Electronic structure ofSi(001)âˆ’c(4Ã—2)analyzed by scanning tunneling spectroscopy andab initiosimulations. Physical Review B, 2006, 73, .	3.2	22
69	Electron transport across carbon nanotube junctions decorated with Au nanoparticles: Density functional calculations. Physical Review B, 2009, 79, .	3.2	22
70	First-principles calculations of lattice-strained core-shell nanocrystals. Physical Review B, 2011, 84, .	3.2	21
71	Using advanced metering infrastructure to characterize residential energy use. Electricity Journal, 2017, 30, 64-70.	2.5	21
72	Orientation dependence of the work function for metal nanocrystals. Journal of Chemical Physics, 2017, 147, 214301.	3.0	21

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73	Estimating the effect of multiple environmental stressors on coral bleaching and mortality. PLoS ONE, 2017, 12, e0175018.	2.5	21
74	Role of dimensionality and quantum confinement in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>-type semiconductor indium phosphide quantum dots. Physical Review B, 2008, 78, .	3.2	20
75	The role of energy storage in accessing remote wind resources in the Midwest. Energy Policy, 2014, 68, 123-131.	8.8	20
76	Real-space pseudopotential calculations of spin-dependent electron transport in magnetic molecular junctions. Physical Review B, 2007, 76, .	3.2	19
77	Quantum confinement, core level shifts, and dopant segregation in P-doped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Si</mml:mtext><mml:mrow><mml:mo>âŸ¨</mml:mo><mml:mrow><mml:mn>110</mml:m Physical Review B, 2010, 82, .	3.2	19
78	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.	5.3	19
79	CO tip functionalization in subatomic resolution atomic force microscopy. Applied Physics Letters, 2015, 107, .	3.3	18
80	Structural and magnetic properties of large cobalt clusters. Physical Review B, 2016, 93, .	3.2	18
81	Estimating the Quantity of Wind and Solar Required To Displace Storage-Induced Emissions. Environmental Science & Technology, 2017, 51, 12988-12997.	10.0	18
82	A perspective on equity implications of net zero energy systems. Energy and Climate Change, 2021, 2, 100047.	4.4	18
83	Real-space pseudopotential method for electron transport properties of nanoscale junctions. Physical Review B, 2006, 73, .	3.2	17
84	Self-purification in Si nanocrystals: An energetics study. Physical Review B, 2010, 82, .	3.2	17
85	<i>Ab initio</i>molecular dynamics simulations of molten Al<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>âˆ’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>Si<mml:m xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>alloys. Physical Review B, 2011, 84, .	3.2	17
86	Repulsive tip tilting as the dominant mechanism for hydrogen bond-like features in atomic force microscopy imaging. Applied Physics Letters, 2016, 108, 193102.	3.3	17
87	Simulating the effect of boron doping in superconducting carbon. Physical Review B, 2018, 97, .	3.2	17
88	Expert assessments on the future of direct current in buildings. Environmental Research Letters, 2018, 13, 074004.	5.2	17
89	Breaking a dative bond with mechanical forces. Nature Communications, 2021, 12, 5635.	12.8	17
90	The food we eat, the air we breathe: a review of the fine particulate matter-induced air quality health impacts of the global food system. Environmental Research Letters, 2021, 16, 103004.	5.2	17

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91	Ab initio molecular dynamics simulations of liquid GaAs. Journal of Chemical Physics, 1998, 109, 7312-7318.	3.0	16
92	Size-dependent induced magnetism in carbon-doped ZnO nanostructures. Applied Physics Letters, 2009, 95, 263108.	3.3	16
93	Time-dependent density functional theory calculations for the Stokes shift in hydrogenated silicon clusters. Physical Review B, 2010, 81, .	3.2	16
94	Hydrogen Storage for Fuel Cell Electric Vehicles: Expert Elicitation and a Levelized Cost of Driving Model. Environmental Science & Technology, 2021, 55, 553-562.	10.0	16
95	Minority-spin polarization and surface magnetic enhancement in Heusler clusters. Physical Review B, 2008, 77, .	3.2	15
96	Keep wind projects close? A case study of distance, culture, and cost in offshore and onshore wind energy siting. Energy Research and Social Science, 2020, 63, 101377.	6.4	15
97	Structural properties of Î±-berlinite (AlPO 4). Physics and Chemistry of Minerals, 1998, 25, 222-226.	0.8	14
98	<i>Ab initio</i>molecular dynamics simulations using a Chebyshev-filtered subspace iteration technique. Physical Review B, 2010, 82, .	3.2	14
99	Improved quasiparticle wave functions and mean field for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml Initialization with the COHSEX operator. Physical Review B, 2014, 90, .	3.2	14
100	Induced seismicity hazard and risk by enhanced geothermal systems: an expert elicitation approach. Environmental Research Letters, 2018, 13, 034004.	5.2	13
101	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.	5.3	13
102	Understanding Cumulative Risk Perception from Judgments and Choices: An Application to Flood Risks. Risk Analysis, 2019, 39, 488-504.	2.7	13
103	Synergistic computational and experimental discovery of novel magnetic materials. Molecular Systems Design and Engineering, 2020, 5, 1098-1117.	3.4	13
104	Theory of spintronic materials. Physica Status Solidi (B): Basic Research, 2006, 243, 2133-2150.	1.5	12
105	Charged dopants in semiconductor nanowires under partially periodic boundary conditions. Physical Review B, 2011, 83, .	3.2	12
106	Electronic properties of mixed-phase graphene/h-BN sheets using real-space pseudopotentials. Physical Review B, 2013, 88, .	3.2	12
107	First-principles study of vibrational modes and Raman spectra in P-doped Si nanocrystals. Physical Review B, 2014, 89, .	3.2	12
108	Insulating titanium oxynitride for visible light photocatalysis. Physical Review B, 2019, 99, .	3.2	12

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109	First principles calculation of the thermodynamic properties of silicon clusters. Theoretical Chemistry Accounts, 1998, 99, 18-28.	1.4	11
110	Ab initiocalculations of the photoelectron spectra of transition metal clusters. Physical Review B, 2005, 71, .	3.2	11
111	An effective one-particle theory for formation energies in doping Si nanostructures. Applied Physics Letters, 2011, 98, 133116.	3.3	11
112	Simulated non-contact atomic force microscopy for GaAs surfaces based on real-space pseudopotentials. Applied Surface Science, 2014, 303, 163-167.	6.1	11
113	Atomically Resolved Elucidation of the Electrochemical Covalent Molecular Grafting Mechanism of Single Layer Graphene. Advanced Materials Interfaces, 2016, 3, 1600196.	3.7	11
114	How Much Are We Saving after All? Characterizing the Effects of Commonly Varying Assumptions on Emissions and Damage Estimates in PJM. Environmental Science & Technology, 2019, 53, 9905-9914.	10.0	11
115	Discrimination of Bond Order in Organic Molecules Using Noncontact Atomic Force Microscopy. Nano Letters, 2019, 19, 5562-5567.	9.1	11
116	Space-Filling Curves for Real-Space Electronic Structure Calculations. Journal of Chemical Theory and Computation, 2021, 17, 4039-4048.	5.3	11
117	Regional and county flows of particulate matter damage in the US. Environmental Research Letters, 2020, 15, 104073.	5.2	11
118	Discovering rare-earth-free magnetic materials through the development of a database. Physical Review Materials, 2020, 4, .	2.4	11
119	Calculated thermodynamic properties of silica polymorphs. Physics and Chemistry of Minerals, 1995, 22, 233.	0.8	10
120	High order forces and nonlocal operators in a Kohnâ€“Sham Hamiltonian. Physical Chemistry Chemical Physics, 2015, 17, 31542-31549.	2.8	10
121	The effect of providing climate and health information on support for alternative electricity portfolios. Environmental Research Letters, 2018, 13, 024026.	5.2	10
122	Trace Element Mass Flow Rates from U.S. Coal Fired Power Plants. Environmental Science & Technology, 2019, 53, 5585-5595.	10.0	10
123	Quantifying the social equity state of an energy system: environmental and labor market equity of the shale gas boom in Appalachia. Environmental Research Letters, 2019, 14, 124072.	5.2	10
124	Support for Emissions Reductions Based on Immediate and Long-term Pollution Exposure in China. Ecological Economics, 2019, 158, 26-33.	5.7	10
125	Magnetism in amorphous carbon. Physical Review Materials, 2018, 2, .	2.4	10
126	Current and Future Estimates of Marginal Emission Factors for Indian Power Generation. Environmental Science & Technology, 2022, 56, 9237-9250.	10.0	10

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127	Algorithms for the electronic and vibrational properties of nanocrystals. Journal of Physics Condensed Matter, 2009, 21, 064207.	1.8	9
128	A first-principles study of the electronic and structural properties of Sb and F doped SnO2 nanocrystals. Journal of Chemical Physics, 2015, 142, 044704.	3.0	9
129	Simulating contrast inversion in atomic force microscopy imaging with real-space pseudopotentials. Physical Review B, 2017, 95, .	3.2	9
130	Economic Viability of a Natural Gas Refueling Infrastructure for Long-Haul Trucks. Journal of Infrastructure Systems, 2019, 25, .	1.8	9
131	Characterizing the association between low-income electric subsidies and the intra-day timing of electricity consumption. Environmental Research Letters, 2020, 15, 094089.	5.2	9
132	Electricity consumption and energy savings potential of video game consoles in the United States. Energy Efficiency, 2012, 5, 531-545.	2.8	8
133	Evaluating the Benefits of Commercial Building Energy Codes and Improving Federal Incentives for Code Adoption. Environmental Science & Technology, 2014, 48, 14121-14130.	10.0	8
134	Ã–ÄŸÃ¼t, Chelikowsky, and Louie Reply:. Physical Review Letters, 1999, 83, 1270-1270.	7.8	7
135	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>-type doping via avoiding the stabilization of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>D</mml:mi><mml:mi>X</mml:mi></mml:mrow></mml:math>centers in InP quantum dots. Physical Review B, 2010, 81, .	3.2	7
136	Comparing the magnitude of simulated residential rebound effects from electric end-use efficiency across the US. Environmental Research Letters, 2014, 9, 074010.	5.2	7
137	Real space pseudopotential calculations for size trends in Ga- and Al-doped zinc oxide nanocrystals with wurtzite and zincblende structures. Journal of Chemical Physics, 2014, 141, 094309.	3.0	7
138	Size dependence of structural stability and magnetization of nickel clusters from real-space pseudopotentials. Physical Review B, 2016, 94, .	3.2	7
139	Climate and Health Benefits of Rapid Coal-to-Gas Fuel Switching in the U.S. Power Sector Offset Methane Leakage and Production Cost Increases. Environmental Science & Technology, 2020, 54, 11494-11505.	10.0	7
140	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: mathvariant="normal">N</mml:mi></mml:mrow></mml:math> clusters. Physical Review Materials, 2018, 2, .	2.4	7
141	Real-space pseudopotential method for calculating magnetocrystalline anisotropy. Physical Review Materials, 2018, 2, .	2.4	7
142	Simulating noncontact atomic force microscopy images. Physical Review Materials, 2019, 3, .	2.4	7
143	Should India Move toward Vehicle Electrification? Assessing Life-Cycle Greenhouse Gas and Criteria Air Pollutant Emissions of Alternative and Conventional Fuel Vehicles in India. Environmental Science & Technology, 2022, 56, 9569-9582.	10.0	7
144	Real-spaceab initiopseudopotential calculations for anion clusters:Fenâˆ’(n=3â€“6). Physical Review B, 2006, 73, .	3.2	6

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145	Ab initiocalculations for the interconversion of optically active defects in amorphous silica. Physical Review B, 2006, 73, .	3.2	6
146	The role of self-purification and the electronic structure of magnetically doped semiconductor nanocrystals. Phase Transitions, 2006, 79, 739-753.	1.3	6
147	Comparing consumer perceptions of appliancesâ€™ electricity use to appliancesâ€™ actual direct-metered consumption. Environmental Research Communications, 2019, 1, 111002.	2.3	6
148	Solar PV as a mitigation strategy for the US education sector. Environmental Research Letters, 2019, 14, 044004.	5.2	6
149	Chemical and steric effects in simulating noncontact atomic force microscopy images of organic molecules on a Cu (111) substrate. Physical Review Materials, 2020, 4, .	2.4	6
150	OPTICAL EXCITATIONS IN NANOSTRUCTURES: APPLICATION OF TIME DEPENDENT DENSITY FUNCTIONAL THEORY TO Si_{n} (n=3-10) CLUSTERS. , 2000, , .		6
151	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></mm 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></mm plus Bethe-Salpeter equationÂcalculations. Physical Review Materials, 2022, 6, .	2.4	6
152	Atomic and Electronic Structure of Germanium Clusters at Finite Temperature Using Finite Difference Methods. Materials Research Society Symposia Proceedings, 1995, 408, 19.	0.1	5
153	Electronic structure and spin polarization of MnGaP. Applied Physics Letters, 2004, 85, 2014-2016.	3.3	5
154	Structural evolution of the Pb/Si(111) interface with metal overlayer thickness. Physical Review B, 2015, 92, .	3.2	5
155	Dynamic data center load response to variability in private and public electricity costs. , 2016, , .		5
156	Computational simulation of subatomic-resolution AFM and STM images for graphene/hexagonal boron nitride heterostructures with intercalated defects. Physical Review B, 2016, 94, .	3.2	5
157	Real-space pseudopotential calculations for simulating noncontact atomic force microscopy images. Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics, 2018, 36, .	1.2	5
158	Effects of Air Emission Externalities on Optimal Ridesourcing Fleet Electrification and Operations. Environmental Science & Technology, 2021, 55, 3188-3200.	10.0	5
159	Quasiparticle energies and dielectric functions of diamond polytypes. Physical Review Materials, 2017, 1, .	2.4	5
160	Enhanced magnetic moments in Mn-doped FeCo clusters owing to ferromagnetic surface Mn atoms. Physical Review Materials, 2019, 3, .	2.4	5
161	Confinement effects in the optical properties of semiconductor nanocrystals. Physica Status Solidi (B): Basic Research, 2006, 243, 2151-2158.	1.5	4
162	On the â€œPreconditioningâ€•Function Used in Planewave DFT Calculations and its Generalization. Communications in Computational Physics, 2015, 18, 167-179.	1.7	4

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163	Real-space pseudopotential study of vibrational properties and Raman spectra in Siâ€“Ge core-shell nanocrystals. Journal of Chemical Physics, 2016, 144, 124110.	3.0	4
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