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	Predicting magnetic anisotropy energies using site-specific spin-orbit coupling energies and machine learning: Application to iron-cobalt nitrides. Physical Review Materials, 2022, 6, .	2.4	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, .	2.4	6
3	Role of carbon in modifying the properties of superconducting hydrogen sulfide. Physical Review Materials, 2022, 6, .	2.4	0
4	Limitations of econometric evaluation of nonrandomized residential energy efficiency programs: A case study of Northern California rebate programs. , 2022, 1, .		1
5	Distributional health impacts of electricity imports in the United States. Environmental Research Letters, 2022, 17, 064011.	5.2	1
6	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
7	Current and Future Estimates of Marginal Emission Factors for Indian Power Generation. Environmental Science & Technology, 2022, 56, 9237-9250.	10.0	10
8	The Great Intergenerational Robbery: A Call for Concerted Action Against Environmental Crises. Annual Review of Environment and Resources, 2022, 47, 1-4.	13.4	2
9	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
10	Do LED lightbulbs save natural gas? Interpreting simultaneous cross-energy program impacts using electricity and natural gas billing data. Environmental Research Communications, 2021, 3, 015003.	2.3	1
11	The impact of Uber and Lyft on vehicle ownership, fuel economy, and transit across U.S. cities. IScience, 2021, 24, 101933.	4.1	25
12	Effects of Air Emission Externalities on Optimal Ridesourcing Fleet Electrification and Operations. Environmental Science & Technology, 2021, 55, 3188-3200.	10.0	5
13	Welfare analysis of the ecological impacts of electricity production in Chile using the sparse multinomial logit model. Ecological Economics, 2021, 184, 107010.	5.7	2
14	Space-Filling Curves for Real-Space Electronic Structure Calculations. Journal of Chemical Theory and Computation, 2021, 17, 4039-4048.	5.3	11
15	Energy Efficiency: What Has Research Delivered in the Last 40 Years?. Annual Review of Environment and Resources, 2021, 46, 135-165.	13.4	41
16	Atomic Fingerprinting of Heteroatoms Using Noncontact Atomic Force Microscopy. Small, 2021, , 2102977.	10.0	3
17	A perspective on equity implications of net zero energy systems. Energy and Climate Change, 2021, 2, 100047.	4.4	18
18	Breaking a dative bond with mechanical forces. Nature Communications, 2021, 12, 5635.	12.8	17

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19	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
20	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
21	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
22	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
23	Prediction of Intrinsic Ferroelectricity and Large Piezoelectricity in Monolayer Arsenic Chalcogenides. Nano Letters, 2020, 20, 8346-8352.	9.1	28
24	Global food system emissions could preclude achieving the 1.5Â° and 2Â°C climate change targets. Science, 2020, 370, 705-708.	12.6	496
25	Optimizing Emissions Reductions from the U.S. Power Sector for Climate and Health Benefits. Environmental Science & Technology, 2020, 54, 7513-7523.	10.0	31
26	Synergistic computational and experimental discovery of novel magnetic materials. Molecular Systems Design and Engineering, 2020, 5, 1098-1117.	3.4	13
27	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
28	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
29	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
30	Regional and county flows of particulate matter damage in the US. Environmental Research Letters, 2020, 15, 104073.	5.2	11
31	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
32	Heavy boron doping in superconducting carbon materials. Physical Review Materials, 2020, 4, .	2.4	3
33	Discovering rare-earth-free magnetic materials through the development of a database. Physical Review Materials, 2020, 4, .	2.4	11
34	Metastable B-doped FeNi compounds for permanent magnets without rare earths. Physical Review Materials, 2020, 4, .	2.4	1
35	Life-cycle greenhouse gas emissions of alternative and conventional fuel vehicles in India. , 2020, , .		4
36	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

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37	Discrimination of Bond Order in Organic Molecules Using Noncontact Atomic Force Microscopy. Nano Letters, 2019, 19, 5562-5567.	9.1	11
38	Comparing consumer perceptions of appliancesâ€™ electricity use to appliancesâ€™ actual direct-metered consumption. Environmental Research Communications, 2019, 1, 111002.	2.3	6
39	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
40	Choice at the pump: measuring preferences for lower-carbon combustion fuels. Environmental Research Letters, 2019, 14, 084035.	5.2	2
41	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
42	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
43	Trace Element Mass Flow Rates from U.S. Coal Fired Power Plants. Environmental Science & Technology, 2019, 53, 5585-5595.	10.0	10
44	Solar PV as a mitigation strategy for the US education sector. Environmental Research Letters, 2019, 14, 044004.	5.2	6
45	Insulating titanium oxynitride for visible light photocatalysis. Physical Review B, 2019, 99, .	3.2	12
46	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
47	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
48	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
49	Cumulative environmental and employment impacts of the shale gas boom. Nature Sustainability, 2019, 2, 1122-1131.	23.7	34
50	Support for Emissions Reductions Based on Immediate and Long-term Pollution Exposure in China. Ecological Economics, 2019, 158, 26-33.	5.7	10
51	Economic Viability of a Natural Gas Refueling Infrastructure for Long-Haul Trucks. Journal of Infrastructure Systems, 2019, 25, .	1.8	9
52	Understanding Cumulative Risk Perception from Judgments and Choices: An Application to Flood Risks. Risk Analysis, 2019, 39, 488-504.	2.7	13
53	Enhanced magnetic moments in Mn-doped FeCo clusters owing to ferromagnetic surface Mn atoms. Physical Review Materials, 2019, 3, .	2.4	5
54	Role of atomic coordination on superconducting properties of boron-doped amorphous carbon. Physical Review Materials, 2019, 3, .	2.4	3

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55	Simulating noncontact atomic force microscopy images. Physical Review Materials, 2019, 3, .	2.4	7
56	A sunny future: expert elicitation of China's solar photovoltaic technologies. Environmental Research Letters, 2018, 13, 034038.	5.2	24
57	Simulating the effect of boron doping in superconducting carbon. Physical Review B, 2018, 97, .	3.2	17
58	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
59	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
60	Assessing the evolution of power sector carbon intensity in the United States. Environmental Research Letters, 2018, 13, 064018.	5.2	52
61	The implications of scope and boundary choice on the establishment and success of metropolitan greenhouse gas reduction targets in the United States. Environmental Research Letters, 2018, 13, 124015.	5.2	4
62	Expert assessments on the future of direct current in buildings. Environmental Research Letters, 2018, 13, 074004.	5.2	17
63	Decarbonizing intraregional freight systems with a focus on modal shift. Environmental Research Letters, 2018, 13, 083001.	5.2	89
64	The effect of providing climate and health information on support for alternative electricity portfolios. Environmental Research Letters, 2018, 13, 024026.	5.2	10
65	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
66	Net-zero emissions energy systems. Science, 2018, 360, .	12.6	1,165
67	Consumersâ€™ perceptions of energy use and energy savings: A literature review. Environmental Research Letters, 2018, 13, 033004.	5.2	34
68	Induced seismicity hazard and risk by enhanced geothermal systems: an expert elicitation approach. Environmental Research Letters, 2018, 13, 034004.	5.2	13
69	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></mm mathvariant="normal">N</mml:mi></mml:mrow></mml:math> clusters. Physical Review Materials, 2018, 2, .	2.4	7
70	Magnetism in amorphous carbon. Physical Review Materials, 2018, 2, .	2.4	10
71	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></m 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></m compounds from first-principles real-space pseudopotentials calculations. Physical Review Materials, 2018, 2, .	2.4	4
72	Real-space pseudopotential method for calculating magnetocrystalline anisotropy. Physical Review Materials, 2018, 2, .	2.4	7

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73	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
74	Lessons from wind policy in Portugal. Energy Policy, 2017, 103, 193-202.	8.8	29
75	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
76	Using advanced metering infrastructure to characterize residential energy use. Electricity Journal, 2017, 30, 64-70.	2.5	21
77	Estimating the Quantity of Wind and Solar Required To Displace Storage-Induced Emissions. Environmental Science & Technology, 2017, 51, 12988-12997.	10.0	18
78	Atomically precise graphene nanoribbon heterojunctions from a single molecular precursor. Nature Nanotechnology, 2017, 12, 1077-1082.	31.5	162
79	Simulating contrast inversion in atomic force microscopy imaging with real-space pseudopotentials. Physical Review B, 2017, 95, .	3.2	9
80	Orientation dependence of the work function for metal nanocrystals. Journal of Chemical Physics, 2017, 147, 214301.	3.0	21
81	Marginal Emissions Factors for Electricity Generation in the Midcontinent ISO. Environmental Science & Technology, 2017, 51, 14445-14452.	10.0	31
82	Formation enthalpies for transition metal alloys using machine learning. Physical Review B, 2017, 95, .	3.2	24
83	Was it worthwhile? Where have the benefits of rooftop solar photovoltaic generation exceeded the cost?. Environmental Research Letters, 2017, 12, 094015.	5.2	45
84	Estimating the effect of multiple environmental stressors on coral bleaching and mortality. PLoS ONE, 2017, 12, e0175018.	2.5	21
85	Quasiparticle energies and dielectric functions of diamond polytypes. Physical Review Materials, 2017, 1, .	2.4	5
86	Atomically Resolved Elucidation of the Electrochemical Covalent Molecular Grafting Mechanism of Single Layer Graphene. Advanced Materials Interfaces, 2016, 3, 1600196.	3.7	11
87	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
88	Real-space pseudopotential method for computing the vibrational Stark effect. Journal of Chemical Physics, 2016, 145, 174111.	3.0	3
89	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
90	Dynamic data center load response to variability in private and public electricity costs. , 2016, , .		5

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91	First-Principles Atomic Force Microscopy Image Simulations with Density Embedding Theory. Nano Letters, 2016, 16, 3242-3246.	9.1	23
92	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
93	Size dependence of structural stability and magnetization of nickel clusters from real-space pseudopotentials. Physical Review B, 2016, 94, .	3.2	7
94	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
95	Structural and magnetic properties of large cobalt clusters. Physical Review B, 2016, 93, .	3.2	18
96	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
97	Ionization of a P-doped Si(111) nanofilm using two-dimensional periodic boundary conditions. Physical Review B, 2015, 91, .	3.2	0
98	Structural evolution of the Pb/Si(111) interface with metal overlayer thickness. Physical Review B, 2015, 92, .	3.2	5
99	On the â€œPreconditioningâ€• Function Used in Planewave DFT Calculations and its Generalization. Communications in Computational Physics, 2015, 18, 167-179.	1.7	4
100	CO tip functionalization in subatomic resolution atomic force microscopy. Applied Physics Letters, 2015, 107, .	3.3	18
101	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
102	Comparison of Life Cycle Greenhouse Gases from Natural Gas Pathways for Light-Duty Vehicles. Energy & Fuels, 2015, 29, 6008-6018.	5.1	58
103	Bulk Energy Storage Increases United States Electricity System Emissions. Environmental Science & Technology, 2015, 49, 3203-3210.	10.0	82
104	High order forces and nonlocal operators in a Kohnâ€“Sham Hamiltonian. Physical Chemistry Chemical Physics, 2015, 17, 31542-31549.	2.8	10
105	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
106	Preface to Special Topic: Selected Contributions to the 32nd International Conference on the Physics of Semiconductors, Austin, 2014. Journal of Applied Physics, 2015, 117, 112701.	2.5	0
107	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
108	A review of learning rates for electricity supply technologies. Energy Policy, 2015, 86, 198-218.	8.8	407

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109	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
110	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
111	Consumer End-Use Energy Efficiency and Rebound Effects. Annual Review of Environment and Resources, 2014, 39, 393-418.	13.4	112
112	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:m Initialization with the COHSEX operator. Physical Review B, 2014, 90, .	3.2	14
113	Labeling energy cost on light bulbs lowers implicit discount rates. Ecological Economics, 2014, 97, 42-50.	5.7	72
114	First-principles study of vibrational modes and Raman spectra in P-doped Si nanocrystals. Physical Review B, 2014, 89, .	3.2	12
115	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
116	Size Effects in the Interface Level Alignment of Dye-Sensitized TiO₂ Clusters. Journal of Physical Chemistry Letters, 2014, 5, 2395-2401.	4.6	28
117	Simulated non-contact atomic force microscopy for GaAs surfaces based on real-space pseudopotentials. Applied Surface Science, 2014, 303, 163-167.	6.1	11
118	The role of energy storage in accessing remote wind resources in the Midwest. Energy Policy, 2014, 68, 123-131.	8.8	20
119	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
120	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
121	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
122	Electronic properties of mixed-phase graphene/h-BN sheets using real-space pseudopotentials. Physical Review B, 2013, 88, .	3.2	12
123	Doping efficiency inn-type InP nanowires. Physical Review B, 2013, 88, .	3.2	3
124	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
125	Electricity consumption and energy savings potential of video game consoles in the United States. Energy Efficiency, 2012, 5, 531-545.	2.8	8
126	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

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127	Edison Revisited: Should we use DC circuits for lighting in commercial buildings?. Energy Policy, 2012, 45, 399-411.	8.8	40
128	First-principles calculations of lattice-strained core-shell nanocrystals. Physical Review B, 2011, 84, .	3.2	21
129	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
130	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
131	<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>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:math>Si<mml: 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
132	An effective one-particle theory for formation energies in doping Si nanostructures. Applied Physics Letters, 2011, 98, 133116.	3.3	11
133	Multidimensional nanoscale materials from fused quantum dots. Physical Review B, 2011, 84, .	3.2	0
134	Charged dopants in semiconductor nanowires under partially periodic boundary conditions. Physical Review B, 2011, 83, .	3.2	12
135	Hybrid density functional study of oligothiophene/ZnO interface for photovoltaics. Physical Review B, 2011, 83, .	3.2	28
136	<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
137	<i>Ab initio</i>molecular dynamics simulations using a Chebyshev-filtered subspace iteration technique. Physical Review B, 2010, 82, .	3.2	14
138	Self-purification in Si nanocrystals: An energetics study. Physical Review B, 2010, 82, .	3.2	17
139	Time-dependent density functional theory calculations for the Stokes shift in hydrogenated silicon clusters. Physical Review B, 2010, 81, .	3.2	16
140	Numerical Methods for Electronic Structure Calculations of Materials. SIAM Review, 2010, 52, 3-54.	9.5	231
141	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: Physical Review B, 2010, 82, .	3.2	19
142	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
143	Electron transport across carbon nanotube junctions decorated with Au nanoparticles: Density functional calculations. Physical Review B, 2009, 79, .	3.2	22
144	Size-dependent induced magnetism in carbon-doped ZnO nanostructures. Applied Physics Letters, 2009, 95, 263108.	3.3	16

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145	Algorithms for the electronic and vibrational properties of nanocrystals. Journal of Physics Condensed Matter, 2009, 21, 064207.	1.8	9
146	Minority-spin polarization and surface magnetic enhancement in Heusler clusters. Physical Review B, 2008, 77, .	3.2	15
147	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
148	Real-space pseudopotential method for first principles calculations of general periodic and partially periodic systems. Physical Review B, 2008, 78, .	3.2	79
149	Transport properties of transition-metal-encapsulated Si cages. Physical Review B, 2008, 77, .	3.2	25
150	Real-space pseudopotential calculations of spin-dependent electron transport in magnetic molecular junctions. Physical Review B, 2007, 76, .	3.2	19
151	Optical excitations in organic molecules, clusters, and defects studied by first-principles Greenâ€™s function methods. Physical Review B, 2006, 73, .	3.2	184
152	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
153	Theory of spintronic materials. Physica Status Solidi (B): Basic Research, 2006, 243, 2133-2150.	1.5	12
154	Confinement effects in the optical properties of semiconductor nanocrystals. Physica Status Solidi (B): Basic Research, 2006, 243, 2151-2158.	1.5	4
155	Self-consistent-field calculations using Chebyshev-filtered subspace iteration. Journal of Computational Physics, 2006, 219, 172-184.	3.8	152
156	Simulating Liquid GeTe. Materials Research Society Symposia Proceedings, 2006, 918, 1.	0.1	0
157	Parallel self-consistent-field calculations via Chebyshev-filtered subspace acceleration. Physical Review E, 2006, 74, 066704.	2.1	145
158	Real-space pseudopotential method for electron transport properties of nanoscale junctions. Physical Review B, 2006, 73, .	3.2	17
159	Real-spaceab initiopseudopotential calculations for anion clusters:Fenâˆ'(n=3â€“6). Physical Review B, 2006, 73, .	3.2	6
160	Electronic structure ofSi(001)âˆ'c(4Ã—2)analyzed by scanning tunneling spectroscopy andab initiosimulations. Physical Review B, 2006, 73, .	3.2	22
161	Ab initiocalculations for the interconversion of optically active defects in amorphous silica. Physical Review B, 2006, 73, .	3.2	6
162	The role of self-purification and the electronic structure of magnetically doped semiconductor nanocrystals. Phase Transitions, 2006, 79, 739-753.	1.3	6

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163	Ab initiocalculations of the photoelectron spectra of transition metal clusters. Physical Review B, 2005, 71, .	3.2	11
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