Emilio Artacho

List of Publications by Year
in descending order

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192 papers	25,708 citations	25034 57 h-index	6131 159 g-index
197 all docs	197 docs citations	197 times ranked	17425 citing authors

#	Article	IF	Citations
1	The SIESTA method forab initioorder-Nmaterials simulation. Journal of Physics Condensed Matter, 2002, 14, 2745-2779.	1.8	9,150
2	Self-consistent order-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>N</mml:mi></mml:math>density-functional calculations for very large systems. Physical Review B, 1996, 53, R10441-R10444.	3.2	2,422
3	Density-functional method for very large systems with LCAO basis sets. International Journal of Quantum Chemistry, 1997, 65, 453-461.	2.0	1,426
4	Numerical atomic orbitals for linear-scaling calculations. Physical Review B, 2001, 64, .	3.2	992
5	Linear-Scaling ab-initio Calculations for Large and Complex Systems. Physica Status Solidi (B): Basic Research, 1999, 215, 809-817.	1.5	922
6	Ab initiostructural, elastic, and vibrational properties of carbon nanotubes. Physical Review B, 1999, 59, 12678-12688.	3.2	854
7	Absence of dc-Conductivity inÎ»-DNA. Physical Review Letters, 2000, 85, 4992-4995.	7.8	602
8	The SIESTA method; developments and applicability. Journal of Physics Condensed Matter, 2008, 20, 064208.	1.8	522
9	Projection of plane-wave calculations into atomic orbitals. Solid State Communications, 1995, 95, 685-690.	1.9	415
10	Lowest Energy Structures of Gold Nanoclusters. Physical Review Letters, 1998, 81, 1600-1603.	7.8	356
11	Transformation of spin information into large electrical signals using carbon nanotubes. Nature, 2007, 445, 410-413.	27.8	325
12	Systematic generation of finite-range atomic basis sets for linear-scaling calculations. Physical Review B, 2002, 66, .	3.2	251
13	Density, structure, and dynamics of water: The effect of van der Waals interactions. Journal of Chemical Physics, 2011, 134, 024516.	3.0	242
14	Structure and Stability of Aluminum Hydroxides:Â A Theoretical Study. Journal of Physical Chemistry B, 2002, 106, 5155-5162.	2.6	241
15	Stiff Monatomic Gold Wires with a Spinning Zigzag Geometry. Physical Review Letters, 1999, 83, 3884-3887.	7.8	235
16	S<scp>iesta</scp>: Recent developments and applications. Journal of Chemical Physics, 2020, 152, 204108.	3.0	229
17	Electronic States in a Finite Carbon Nanotube: A One-Dimensional Quantum Box. Physical Review Letters, 1999, 82, 3520-3523.	7.8	173
18	Metallic bonding and cluster structure. Physical Review B, 2000, 61, 5771-5780.	3.2	163

#	Article	IF	Citations
19	Analysis of atomic orbital basis sets from the projection of plane-wave results. Journal of Physics Condensed Matter, 1996, 8, 3859-3880.	1.8	161
20	Do Thiols Merely Passivate Gold Nanoclusters?. Physical Review Letters, 2000, 85, 5250-5251.	7.8	158
21	Electronic Stopping Power in LiF from First Principles. Physical Review Letters, 2007, 99, 235501.	7.8	157
22	Network equilibration and first-principles liquid water. Journal of Chemical Physics, 2004, 121, 11136.	3.0	155
23	Ferrielectric Twin Walls in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CaTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2008, 101, 097602.	7.8	148
24	Surface defects and conduction in polar oxide heterostructures. Physical Review B, 2011, 83, .	3.2	145
25	The origin of two-dimensional electron gases at oxide interfaces: insights from theory. Journal of Physics Condensed Matter, 2014, 26, 143201.	1.8	140
26	Nonadiabatic Forces in Ion-Solid Interactions: The Initial Stages of Radiation Damage. Physical Review Letters, 2012, 108, 213201.	7.8	138
27	The flexoelectricity of barium and strontium titanates from first principles. Journal of Physics Condensed Matter, 2010, 22, 112201.	1.8	130
28	Electronic Stopping Power in Gold: The Role of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>d</mml:mi></mml:math>Electrons and the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi mathvariant="bold">H</mml:mi><mml:mo>/</mml:mo><mml:mi>He</mml:mi></mml:math>Anomaly. Physical Review Letters, 2012, 108, 225504.	7.8	125
29	First-principles study of structural, elastic, and bonding properties of pyrochlores. Physical Review B, 2005, 72, .	3.2	119
30	Proposal for symmetric dimers at the Si(100)-2Ã—1 surface. Physical Review Letters, 1989, 62, 2491-2494.	7.8	118
31	Seeing molecular orbitals. Chemical Physics Letters, 2000, 321, 78-82.	2.6	117
32	How the nature of the chemical bond governs resistance to amorphization by radiation damage. Physical Review B, 2005, 71, .	3.2	104
33	Systematicab initiostudy of the electronic and magnetic properties of different pure and mixed iron systems. Physical Review B, 2000, 61, 13639-13646.	3.2	98
34	Small Polarons in Dry DNA. Physical Review Letters, 2003, 91, 108105.	7.8	94
35	Self-consistent density-functional calculations of the geometries, electronic structures, and magnetic moments of Ni-Al clusters. Physical Review B, 1999, 60, 2020-2024.	3.2	88
36	Electrons and Hydrogen-Bond Connectivity in Liquid Water. Physical Review Letters, 2006, 96, 016404.	7.8	88

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37	Electrons in dry DNA from density functional calculations. Molecular Physics, 2003, 101, 1587-1594.	1.7	87
38	New Superhard Phases for Three-DimensionalC60-based Fullerites. Physical Review Letters, 2000, 85, 2328-2331.	7.8	85
39	Density-functional study of charge doping inWO3. Physical Review B, 2004, 70, .	3.2	84
40	Structural changes on supercooling liquid silicon. Applied Physics Letters, 2003, 83, 4734-4736.	3.3	82
41	Single adatom adsorption and diffusion onSi(111)â˜(7Ã—7)surfaces:â€ƒScanning tunneling microscopy and first-principles calculations. Physical Review B, 2003, 67, .	3.2	78
42	Linear Scaling DFT Calculations with Numerical Atomic Orbitals. Materials Research Society Symposia Proceedings, 2001, 677, 961.	0.1	77
43	Stopping power beyond the adiabatic approximation. Scientific Reports, 2017, 7, 2618.	3.3	77
44	Nature of the Structural Transformations in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Glass under High Pressure. Physical Review Letters, 2008, 101, 035702.	7.8	76
45	Quantum mechanical calculations of dioctahedral 2:1 phyllosilicates: Effect of octahedral cation distributions in pyrophyllite, illite, and smectite. American Mineralogist, 2002, 87, 958-965.	1.9	73
46	Topology of the polarization field in ferroelectric nanowires from first principles. Physical Review B, 2010, 81, .	3.2	73
47	Core Electrons in the Electronic Stopping of Heavy Ions. Physical Review Letters, 2018, 121, 116401.	7.8	72
48	Energetics of the oxidation and opening of a carbon nanotube. Physical Review B, 1999, 60, R2208-R2211.	3.2	69
49	Atomistic simulations of resistance to amorphization by radiation damage. Physical Review B, 2006, 73, .	3.2	68
50	Polarons in Carbon Nanotubes. Physical Review Letters, 2001, 86, 3372-3375.	7.8	67
51	Oxide superlattices with alternating<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>interfaces. Physical Review B, 2009, 80, .	3.2	65
52	Probing Surface and Bulk Electrochemical Processes on the LaAlO₃â€“SrTiO₃ Interface. ACS Nano, 2012, 6, 3841-3852.	14.6	65
53	Nonorthogonal basis sets in quantum mechanics: Representations and second quantization. Physical Review A, 1991, 43, 5770-5777.	2.5	64
54	Tailoring Band Gap and Hardness by Intercalation: Anab initioStudy ofI8@Siâ˜46and Related Doped Clathrates. Physical Review Letters, 2001, 87, 206405.	7.8	64

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55	Trapping of oxygen vacancies in the twin walls of perovskite. Physical Review B, 2010, 81, .	3.2	64
56	Structural and configurational properties of nanoconfined monolayer ice from first principles. Scientific Reports, 2016, 6, 18651.	3.3	61
57	Molecular and Electronic Structure of the Peptide Subunit of Geobacter sulfurreducens Conductive Pili from First Principles. Journal of Physical Chemistry A, 2012, 116, 8023-8030.	2.5	58
58	Electronic stopping power in a narrow band gap semiconductor from first principles. Physical Review B, 2015, 91, .	3.2	57
59	Chemistry on the computer. Physics Today, 2008, 61, 58-63.	0.3	56
60	Interstitial oxygen in germanium and silicon. Physical Review B, 1997, 56, 3820-3833.	3.2	55
61	Neutral self-defects in a silica model: A first-principles study. Physical Review B, 2005, 71, .	3.2	55
62	Mechanical architecture and folding of E. coli type 1 pilus domains. Nature Communications, 2018, 9, 2758.	12.8	55
63	Room temperature compressibility and diffusivity of liquid water from first principles. Journal of Chemical Physics, 2013, 139, 194502.	3.0	54
64	Structure and thermal stability of gold nanoclusters: The Au38 case. European Physical Journal D, 1999, 9, 211-215.	1.3	52
65	Structural Relaxations in Electronically Excited Poly(para-phenylene). Physical Review Letters, 2004, 93, 116401.	7.8	49
66	Atomistic and electronic structure of antisite defects in yttrium aluminum garnet: Density-functional study. Physical Review B, 2009, 80, .	3.2	45
67	Zigzag equilibrium structure in monatomic wires. Surface Science, 2001, 482-485, 1261-1265.	1.9	42
68	Enhanced Configurational Entropy in High-Density Nanoconfined Bilayer Ice. Physical Review Letters, 2016, 116, 085901.	7.8	42
69	First-Principles Infrared Spectrum of Nitric Acid and Nitric Acid Monohydrate Crystals. Journal of Physical Chemistry A, 2004, 108, 10535-10541.	2.5	41
70	van der Waals interaction in magnetic bilayer graphene nanoribbons. Physical Review B, 2012, 85, .	3.2	41
71	Ferrodistortive Instability at the (001) Surface of Half-Metallic Manganites. Physical Review Letters, 2007, 99, 226101.	7.8	40
72	Atomic layering at the liquid silicon surface: A first-principles simulation. Physical Review B, 1999, 60, R16283-R16286.	3.2	39

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73	The structure and dynamics of crystalline durene by neutron scattering and numerical modelling using density functional methods. Chemical Physics, 2000, 261, 189-203.	1.9	39
74	Energetics of intrinsic point defects inZrSiO4. Physical Review B, 2005, 71, .	3.2	39
75	Novel Structural Features of CDK Inhibition Revealed by an ab Initio Computational Method Combined with Dynamic Simulations. Journal of Medicinal Chemistry, 2006, 49, 5141-5153.	6.4	37
76	Electrochemical ferroelectric switching: Origin of polarization reversal in ultrathin films. Physical Review B, 2012, 85, .	3.2	37
77	Bonding and diffusion of Ba on a Si(001) reconstructed surface. Physical Review B, 1999, 60, 4968-4971.	3.2	36
78	Fermi surfaces and orbital polarization in superconducting<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>CeO</mml:mi><mml:mrow><mml:mn>0.5<mathvariant="normal">F</mml:mi><mml:mrow><mml:mn>0.5</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mi>BiS</mml:m by angle-resolved photoemission spectroscopy. Physical Review B, 2015, 92, .	3.2	36
79	Hybrid DNA-gold nanostructured materials: anab initioapproach. Nanotechnology, 2001, 12, 126-131.	2.6	35
80	Radiation damage effects in the perovskiteCaTiO3and resistance of materials to amorphization. Physical Review B, 2004, 70, .	3.2	35
81	Linear-Scaling ab-initio Calculations for Large and Complex Systems. , 1999, 215, 809.		35
82	Electron density in the peptide bonds of crambin. Solid State Communications, 2000, 116, 395-400.	1.9	34
83	Ab initiocalculations and scanning tunneling microscopy experiments of theSi(111)â3(7Ã—3)â3Pbsurface. Physical Review B, 2002, 66, .	3.2	34
84	Two-dimensional electron gas at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>PbTi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mo>/</mml:mo><mml:mi>SrTi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>interface: Anab initiostudy. Physical Review B, 2015, 92, .	3.2	34
85	Density functionals and half-metallicity in La2/3Sr1/3MnO3. Physica Status Solidi (A) Applications and Materials Science, 2006, 203, 1437-1441.	1.8	33
86	Interstitial O isotope effects in silicon. Journal of Physics Condensed Matter, 1995, 7, 7077-7085.	1.8	32
87	Two exchange-correlation functionals compared for first-principles liquid water. Molecular Simulation, 2005, 31, 361-366.	2.0	32
88	Electronic stopping power of H and He in Al and LiF from first principles. Nuclear Instruments & Methods in Physics Research B, 2013, 303, 59-61.	1.4	32
89	Spin polarization and dimer buckling at the Si(100)-2Ã—1 surface. Physical Review B, 1990, 42, 11310-11316.	3.2	30
90	Experimental and Theoretical Electron Density Studies in Large Molecules:Â NAD+, Î²-Nicotinamide Adenine Dinucleotide. Journal of Physical Chemistry B, 2003, 107, 9109-9121.	2.6	30

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91	Model of two-dimensional electron gas formation at ferroelectric interfaces. Physical Review B, 2015, 92, .	3.2	30
92	Microscopic structure of the discommensurate phases in Ge(111)/Ga. II. Domain superstructure and discommensurations. Physical Review B, 1995, 51, 9965-9972.	3.2	29
93	Geometry and quantum delocalization of interstitial oxygen in silicon. Physical Review B, 1995, 51, 7862-7865.	3.2	28
94	The intrinsic elasticity of twin walls: Ferrielectric twin walls in ferroelastic CaTiO3. Applied Physics Letters, 2009, 94, 081903.	3.3	28
95	One-dimensional half-metallic interfaces of two-dimensional honeycomb insulators. Physical Review B, 2013, 88, .	3.2	28
96	Optimal finite-range atomic basis sets for liquid water and ice. Journal of Physics Condensed Matter, 2013, 25, 435504.	1.8	25
97	Nonparametrized tight-binding method for local and extended defects in homopolar semiconductors. Physical Review B, 1991, 44, 6169-6187.	3.2	24
98	Intrinsic point defects and volume swelling inZrSiO4under irradiation. Physical Review B, 2004, 70, .	3.2	24
99	Electronic stopping in insulators: a simple model. Journal of Physics Condensed Matter, 2007, 19, 275211.	1.8	24
100	Resistive and rectifying effects of pulling gold atoms at thiol-gold nanocontacts. Physical Review B, 2007, 75, .	3.2	22
101	First-principles calculations of structural changes in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>B</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mtext> under pressure. Physical Review B, 2008, 78, .	3.2	22
102	Atomic configuration of H-based complexes in silicon. Solid State Communications, 1989, 72, 393-396.	1.9	21
103	Ices of CO₂/H₂O Mixtures. Reflectionâ^'Absorption IR Spectroscopy and Theoretical Calculations. Journal of Physical Chemistry A, 2008, 112, 457-465.	2.5	21
104	Proposal of a One-Dimensional Electron Gas in the Steps at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>LaAlO</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mtext mathvariant="normal">â^'</mml:mtext><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Interf Physical Review Letters, 2012, 108, 166802.	7.8	21
105	Microscopic structure of the discommensurate phases in Ge(111)/Ga. I. Atomic structure within domains. Physical Review B, 1995, 51, 9952-9964.	3.2	20
106	Model Hessian for accelerating first-principles structure optimizations. Physical Review B, 2003, 67, .	3.2	19
107	Oxygen neutral defects in silica: Origin of the distribution of the formation energies. Europhysics Letters, 2004, 66, 680-686.	2.0	19
108	Knock-on damage in bilayer graphene: Indications for a catalytic pathway. Physical Review B, 2013, 88, .	3.2	19

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109	Anisotropy of electronic stopping power in graphite. Physical Review B, 2019, 100, .	3.2	19
110	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	3.0	19
111	Dispersion interactions in room-temperature ionic liquids: Results from a non-empirical density functional. Journal of Chemical Physics, 2011, 135, 154505.	3.0	18
112	The net charge at interfaces between insulators. Journal of Physics Condensed Matter, 2011, 23, 081001.	1.8	18
113	Electrostatic versus polarization effects in the adsorption of aromatic molecules of varied polarity on an insulating hydrophobic surface. Journal of Physics Condensed Matter, 2008, 20, 035215.	1.8	16
114	Quantum mechanics in an evolving Hilbert space. Physical Review B, 2017, 95, .	3.2	16
115	Electron correlation in the Si(1 0 0) surface. Surface Science, 2001, 482-485, 458-463.	1.9	15
116	Interplay between theory and experiment in solid state inorganic chemistry. Journal of Materials Chemistry, 2001, 11, 1-10.	6.7	15
117	Simulations of minerals using density-functional theory based on atomic orbitals for linear scaling. Physics and Chemistry of Minerals, 2004, 31, 12-21.	0.8	15
118	Electronic and magnetic properties of superconductingLnO_{1â^'x}F_xBiS₂(Lnâ€‰â€‰â€‰â€‰a,) Tj ETQ	1.8	15
119	Continuous melting through a hexatic phase in confined bilayer water. Physical Review E, 2016, 93, 062137.	2.1	15
120	First-principles characterization of single-electron polaron in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>WO</mml:mi><mml:mn>3</mml:mn></mml:msub></mm Physical Review Research, 2020, 2, .	3.6	15
121	O isotope effects and vibration-rotation lines of interstitial oxygen in germanium. Physical Review B, 2000, 62, 10165-10172.	3.2	14
122	First principles study of the adsorption of C60 on Si(1 1 1). Surface Science, 2001, 482-485, 39-43.	1.9	14
123	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="italic">Ab</mml:mi></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="italic">initio</mml:mi></mml:math>calculation of the shock Hugoniot of bulk silicon. Physical Review B, 2016, 93, .	3.2	14
124	Surface energy and stability of stress-driven discommensurate surface structures. Physical Review B, 1995, 52, 16373-16376.	3.2	13
125	Application of local-spin-density approximation toaâ^'Siand tetrahedralaâ^'C. Physical Review B, 1999, 60, 10594-10597.	3.2	13
126	Effects of stoichiometric doping in superconducting Bi-O-S compounds. Journal of Physics Condensed Matter, 2015, 27, 135501.	1.8	13

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127	Surface electronic structure of metastable FeSi(CsCl)(111) epitaxially grown on Si(111). Physical Review B, 1997, 55, R16065-R16068.	3.2	12
128	Comment on â€œIdentifying Molecular Orientation of IndividualC60on aSi(111)â˜'(7Ã—7)Surfaceâ€• Physical Review Letters, 2000, 85, 2653-2653.	7.8	12
129	Comparison between plane-wave and linear-scaling localized basis sets for structural calculations of microporous molecular sieves. Physical Review B, 2003, 68, .	3.2	12
130	Short-range repulsive interatomic interactions in energetic processes in solids. Physical Review B, 2004, 70, .	3.2	12
131	Critical assessment of classical potentials for MgSiO3 perovskite with application to thermal conductivity calculations. Physics of the Earth and Planetary Interiors, 2012, 210-211, 75-89.	1.9	12
132	Electrostatics and domains in ferroelectric superlattices. Royal Society Open Science, 2020, 7, 201270.	2.4	12
133	Open fermionic quantum systems. Physical Review B, 1993, 47, 1190-1198.	3.2	11
134	Surface structures of Si(111)/Ga. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1994, 70, 731-745.	0.6	11
135	Low-energy quantum dynamics of atoms at defects; interstitial oxygen in silicon. Journal of Physics Condensed Matter, 1997, 9, 3107-3116.	1.8	11
136	Electronic structure computations of Newton Black Films. Journal of Materials Chemistry, 2010, 20, 10351.	6.7	11
137	Quasi-parity-conserving octahedral model for (H,Be) and (D,Be) tunneling complexes in silicon. Physical Review B, 1991, 43, 12507-12511.	3.2	10
138	Surface layering and local structure in liquid surfaces. Surface Science, 2001, 482-485, 1314-1318.	1.9	10
139	Calculation of the effect of intrinsic point defects and volume swelling in the nuclear magnetic resonance spectra of ZrSiO4. Molecular Simulation, 2005, 31, 349-354.	2.0	10
140	Radiation damage in the bulk and at the surface. Molecular Simulation, 2005, 31, 355-359.	2.0	10
141	Bulk properties and near-critical behaviour of SiO2 fluid. Earth and Planetary Science Letters, 2018, 491, 11-20.	4.4	10
142	Water radiolysis by low-energy carbon projectiles from first-principles molecular dynamics. PLoS ONE, 2017, 12, e0171820.	2.5	10
143	Mixed Approach to Incorporate Self-Consistency into Order-N LCAO Methods. Materials Research Society Symposia Proceedings, 1995, 408, 85.	0.1	9
144	Matrix-Induced Isotope Shift of a Vibrational Mode of Interstitial Oxygen in Germanium. Materials Science Forum, 1997, 258-263, 41-46.	0.3	9

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145	Characterization of electrodeposited zinc oxide/tetrasulphonatedcopper phthalocyanines (ZnO/Ts-CuPc) hybrid films and their photoelectrochemical properties. Journal of Electroanalytical Chemistry, 2011, 653, 86-92.	3.8	9
146	Prediction of equilibrium isotopic fractionation of the gypsum/bassanite/water system using first-principles calculations. Geochimica Et Cosmochimica Acta, 2019, 244, 1-11.	3.9	9
147	Ab initio electronic stopping power for protons in Ga _{0.5} In _{0.5} P/GaAs/Ge triple-junction solar cells for space applications. Royal Society Open Science, 2020, 7, 200925.	2.4	9
148	First-principles molecular dynamics simulations of the interaction of ionic projectiles with liquid water and ice. , 2008, , .		8
149	eScience for molecular-scale simulations and the e Minerals project. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2009, 367, 967-985.	3.4	8
150	Linearâ€"Scaling Calculations of Linear and Nonlinear Optical Properties of [60]fullerene Derivatives. , 2009, , .		7
151	Simulations of water nano-confined between corrugated planes. Journal of Chemical Physics, 2017, 147, 194509.	3.0	7
152	Efficient ab initio calculation of electronic stopping in disordered systems via geometry pre-sampling: Application to liquid water. Journal of Chemical Physics, 2020, 153, 034113.	3.0	7
153	The phase diagram of annealed Ge(111)/Ga. Physica Status Solidi A, 1995, 148, 191-212.	1.7	6
154	Metallic surface reconstruction driven by frustrated antiferromagnetism. Physical Review B, 1999, 59, R705-R708.	3.2	6
155	Reader-appeal should not outweigh merit of research. Nature, 2006, 439, 534-534.	27.8	6
156	Electronic heat transport versus atomic heating in irradiated short metallic nanowires. Physical Review B, 2019, 100, .	3.2	6
157	A computational exploration of cation locations in high- silica Ca-Chabazite. Studies in Surface Science and Catalysis, 2000, 128, 89-98.	1.5	5
158	Comparison of dispersion-corrected exchange-correlation functionals using atomic orbitals. Physical Review B, 2019, 100, .	3.2	5
159	Semi-empirical and linear-scaling DFT methods to characterize duplex DNA and G-quadruplexes in the presence of interacting small molecules. Physical Chemistry Chemical Physics, 2022, 24, 11510-11519.	2.8	5
160	Theory of Interstitial Oxygen in Silicon and Germanium. Materials Science Forum, 1995, 196-201, 103-108.	0.3	4
161	Ab initio study of atomic oxygen adsorption on the Si surface. Physica B: Condensed Matter, 2001, 308-310, 329-332.	2.7	4
162	Heating electrons with ion irradiation: A first-principles approach. Nuclear Instruments & Methods in Physics Research B, 2009, 267, 590-593.	1.4	4

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163	Comment on â€œQuantum Mechanics in Metric Space: Wave Functions and their Densitiesâ€. Physical Review Letters, 2011, 107, 188901; discussion 188902.	7.8	4
164	Structure and thermal stability of gold nanoclusters: The Au38 case. , 1999, , 211-215.		4
165	Floquet theory for the electronic stopping of projectiles in solids. Physical Review Research, 2020, 2, .	3.6	4
166	Inelastic scattering of electrons in water from first principles: cross sections and inelastic mean free path for use in Monte Carlo track-structure simulations of biological damage. Royal Society Open Science, 2022, 9, .	2.4	4
167	Electronic Structure Calculations with Localized Orbitals: The Siesta Method. , 2005, , 77-91.		3
168	Preface: phys. stat. sol. (b) 243/5. Physica Status Solidi (B): Basic Research, 2006, 243, 971-972.	1.5	3
169	Prediction of the near-IR spectra of ices by ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2019, 21, 9433-9440.	2.8	2
170	Numerical integration of quantum time evolution in a curved manifold. Physical Review Research, 2021, 3, .	3.6	2
171	Bragg's additivity rule and core and bond model studied by real-time TDDFT electronic stopping simulations: The case of water vapor. Radiation Physics and Chemistry, 2022, 193, 109961.	2.8	2
172	Weakening of bonds: Discussion of two different mechanisms. Solid State Communications, 1987, 62, 113-115.	1.9	1
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