Peter Zapol

List of Publications by Year
in descending order

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155	12,181	34105 52	25787 108
papers	citations	h-index	g-index

157	157	157	15746
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Measurements of near-ultimate strength for multiwalled carbon nanotubes and irradiation-induced crosslinking improvements. Nature Nanotechnology, 2008, 3, 626-631.	31.5	972
2	Nanostructured transition metal dichalcogenide electrocatalysts for CO ₂ reduction in ionic liquid. Science, 2016, 353, 467-470.	12.6	778
3	Subnanometre platinum clusters as highly activeÂand selective catalysts for the oxidative dehydrogenation of propane. Nature Materials, 2009, 8, 213-216.	27.5	725
4	Hierarchical Nanoassembly of MoS₂/Co₉S₈/Ni₃S₂/Ni as a Highly Efficient Electrocatalyst for Overall Water Splitting in a Wide pH Range. Journal of the American Chemical Society, 2019, 141, 10417-10430.	13.7	653
5	Dynamic stability of active sites in hydr(oxy)oxides for the oxygen evolution reaction. Nature Energy, 2020, 5, 222-230.	39.5	540
6	Synthesis and characterization of highly-conducting nitrogen-doped ultrananocrystalline diamond films. Applied Physics Letters, 2001, 79, 1441-1443.	3.3	465
7	Role of Water and Carbonates in Photocatalytic Transformation of CO₂ to CH₄ on Titania. Journal of the American Chemical Society, 2011, 133, 3964-3971.	13.7	416
8	Carbon Dioxide Conversion to Methanol over Size-Selected Cu₄ Clusters at Low Pressures. Journal of the American Chemical Society, 2015, 137, 8676-8679.	13.7	299
9	Tight-binding molecular-dynamics simulation of impurities in ultrananocrystalline diamond grain boundaries. Physical Review B, 2001, 65, .	3.2	267
10	A model for the phase stability of arbitrary nanoparticles as a function of size and shape. Journal of Chemical Physics, 2004, 121, 4276-4283.	3.0	253
11	Assessment of Gaussian-3 and Density Functional Theories for Enthalpies of Formation of C1â^'C16 Alkanes. Journal of Physical Chemistry A, 2000, 104, 5850-5854.	2.5	231
12	Lyotropic Liquid-Crystalline Gel Formation in a Room-Temperature Ionic Liquid. Langmuir, 2002, 18, 7258-7260.	3.5	229
13	Dopantâ€Dependent Stability of Garnet Solid Electrolyte Interfaces with Lithium Metal. Advanced Energy Materials, 2019, 9, 1803440.	19.5	217
14	Computational Studies of Catechol and Water Interactions with Titanium Oxide Nanoparticles. Journal of Physical Chemistry B, 2003, 107, 11419-11427.	2.6	208
15	Tailoring the Edge Structure of Molybdenum Disulfide toward Electrocatalytic Reduction of Carbon Dioxide. ACS Nano, 2017, 11, 453-460.	14.6	208
16	Effects of particle morphology and surface hydrogenation on the phase stability ofTiO2. Physical Review B, 2004, 70, .	3.2	200
17	Modeling the Morphology and Phase Stability of TiO2 Nanocrystals in Water. Journal of Chemical Theory and Computation, 2005, 1, 107-116.	5.3	191
18	Cathode Based on Molybdenum Disulfide Nanoflakes for Lithiumâ€“Oxygen Batteries. ACS Nano, 2016, 10, 2167-2175.	14.6	184

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19	Microporous polyphenylenes with tunable pore size for hydrogen storage. Chemical Communications, 2010, 46, 4547.	4.1	170
20	Charge Transfer Across the Nanocrystalline-DNA Interface:Â Probing DNA Recognition. Nano Letters, 2004, 4, 1017-1023.	9.1	164
21	A Theoretical Study of CO₂ Anions on Anatase (101) Surface. Journal of Physical Chemistry C, 2010, 114, 21474-21481.	3.1	159
22	Revisiting the Corrosion of the Aluminum Current Collector in Lithium-Ion Batteries. Journal of Physical Chemistry Letters, 2017, 8, 1072-1077.	4.6	156
23	Dynamically Stable Active Sites from Surface Evolution of Perovskite Materials during the Oxygen Evolution Reaction. Journal of the American Chemical Society, 2021, 143, 2741-2750.	13.7	156
24	Copper Cluster Size Effect in Methanol Synthesis from CO₂. Journal of Physical Chemistry C, 2017, 121, 10406-10412.	3.1	144
25	Computational screening of dopants for photocatalytic two-electron reduction of CO2 on anatase (101) surfaces. Energy and Environmental Science, 2012, 5, 6196.	30.8	138
26	Shape-Dependent Activity of Platinum Array Catalyst. Journal of the American Chemical Society, 2009, 131, 5732-5733.	13.7	134
27	Photoredox Reactions and the Catalytic Cycle for Carbon Dioxide Fixation and Methanogenesis on Metal Oxides. Journal of Physical Chemistry C, 2012, 116, 9450-9460.	3.1	129
28	Shaping Nanometer-Scale Architecture Through Surface Chemistry. Advanced Materials, 2005, 17, 965-971.	21.0	125
29	The effect of nitrogen addition to Ar/CH4 plasmas on the growth, morphology and field emission of ultrananocrystalline diamond. Diamond and Related Materials, 2002, 11, 43-48.	3.9	121
30	2D Copper Tetrahydroxyquinone Conductive Metalâ€“Organic Framework for Selective CO₂ Electrocatalysis at Low Overpotentials. Advanced Materials, 2021, 33, e2004393.	21.0	120
31	Vacancy-Mediated Anion Photosegregation Kinetics in Mixed Halide Hybrid Perovskites: Coupled Kinetic Monte Carlo and Optical Measurements. ACS Energy Letters, 2018, 3, 2321-2328.	17.4	119
32	Predicting the Energetics, Phase Stability, and Morphology Evolution of Faceted and Spherical Anatase Nanocrystals. Journal of Physical Chemistry B, 2004, 108, 18435-18440.	2.6	115
33	Anatase and rutile surfaces with adsorbates representative of acidic and basic conditions. Surface Science, 2005, 582, 173-188.	1.9	107
34	Diffusion mechanisms of native point defects in rutileTiO2:Ab initiototal-energy calculations. Physical Review B, 2007, 75, .	3.2	107
35	Ab Initio and Density Functional Study of the Activation Barrier for Ethane Cracking in Cluster Models of Zeolite H-ZSM-5. Journal of Physical Chemistry B, 2000, 104, 1944-1949.	2.6	106
36	Avalanching strain dynamics during the hydriding phase transformation in individual palladium nanoparticles. Nature Communications, 2015, 6, 10092.	12.8	87

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37	Catalytic Fe-xN Sites in Carbon Nanotubes. Journal of Physical Chemistry C, 2009, 113, 21629-21634.	3.1	83
38	Atomistic simulations of amorphous alumina surfaces. Physical Review B, 2006, 74, .	3.2	81
39	Three-dimensional imaging of dislocation dynamics during the hydriding phase transformation. Nature Materials, 2017, 16, 565-571.	27.5	81
40	Charge Distribution and Stability of Charged Carbon Nanotubes. Physical Review Letters, 2002, 89, 255503.	7.8	79
41	Interfacial control of oxygen vacancy doping and electrical conduction in thin film oxide heterostructures. Nature Communications, 2016, 7, 11892.	12.8	77
42	Oxidative Decomposition of Methanol on Subnanometer Palladium Clusters: The Effect of Catalyst Size and Support Composition. Journal of Physical Chemistry C, 2010, 114, 10342-10348.	3.1	76
43	Carbon Ad-Dimer Defects in Carbon Nanotubes. Physical Review Letters, 2006, 96, 075506.	7.8	70
44	Density functional study of the TiO2â€“dopamine complex. Chemical Physics Letters, 2005, 406, 306-311.	2.6	67
45	Firstâ€Principles Study of Hydrolysis Reaction Barriers in a Sodium Borosilicate Glass. International Journal of Applied Glass Science, 2013, 4, 395-407.	2.0	66
46	An interatomic potential study of the properties of gallium nitride. Journal of Physics Condensed Matter, 1997, 9, 9517-9525.	1.8	65
47	High-Voltage Phosphate Cathodes for Rechargeable Ca-Ion Batteries. ACS Energy Letters, 2020, 5, 3203-3211.	17.4	65
48	Computational studies of electrochemical CO₂ reduction on subnanometer transition metal clusters. Physical Chemistry Chemical Physics, 2014, 16, 26584-26599.	2.8	62
49	Theoretical Studies on Nanocrystalline Diamond:â€‰ Nucleation by Dicarbon and Electronic Structure of Planar Defects. Journal of Physical Chemistry B, 1999, 103, 5459-5467.	2.6	58
50	Ab initioprediction of GaN (101Â¯0) and (110) anomalous surface relaxation. Physical Review B, 1996, 53, R4209-R4212.	3.2	56
51	Quantum Chemical Study of Mechanisms for Oxidative Dehydrogenation of Propane on Vanadium Oxide. Journal of Physical Chemistry B, 2006, 110, 8363-8371.	2.6	54
52	Modeling the structure and electronic properties ofTiO2nanoparticles. Physical Review B, 2006, 73, .	3.2	53
53	Structure and Morphology of Hydroxylated Amorphous Alumina Surfaces. Journal of Physical Chemistry C, 2007, 111, 7422-7429.	3.1	53
54	Carbon dimers on the diamond (100) surface:â€,â€,Growth and nucleation. Physical Review B, 2003, 68, .	3.2	52

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55	Monomeric Vanadium Oxide on a Î¸-Al₂O₃Support: A Combined Experimental/Theoretical Study. Journal of Physical Chemistry C, 2009, 113, 8836-8843.	3.1	52
56	High Voltage Mg-Ion Battery Cathode via a Solid Solution Crâ€“Mn Spinel Oxide. Chemistry of Materials, 2020, 32, 6577-6587.	6.7	48
57	High Capacity for Mg²⁺ Deintercalation in Spinel Vanadium Oxide Nanocrystals. ACS Energy Letters, 2020, 5, 2721-2727.	17.4	48
58	Atomistic calculations of defects in ZnGeP2. Journal of Applied Physics, 1996, 79, 671.	2.5	45
59	Tailoring the Load Carrying Capacity of MWCNTs Through Inter-shell Atomic Bridging. Experimental Mechanics, 2009, 49, 169-182.	2.0	45
60	Heteroatom-Transfer Coupled Photoreduction and Carbon Dioxide Fixation on Metal Oxides. Journal of Physical Chemistry C, 2012, 116, 9461-9471.	3.1	45
61	Ab initio study of hydrogen adsorption on the ZnO (101Ì„0) surface. Surface Science, 1999, 422, 1-7.	1.9	43
62	New Class of Electrocatalysts Based on 2D Transition Metal Dichalcogenides in Ionic Liquid. Advanced Materials, 2019, 31, e1804453.	21.0	43
63	Shape of Platinum Nanoparticles Supported on SrTiO₃:â€‰ Experiment and Theory. Journal of Physical Chemistry C, 2007, 111, 14782-14789.	3.1	42
64	Transport properties of n-type ultrananocrystalline diamond films. Physical Review B, 2006, 74, .	3.2	40
65	First-principles study of the atomic and electronic structures of misfit-layered calcium cobaltite		

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73	Theoretical study of nonpolar surfaces of aluminum nitride: Zinc blende (110) and wurtzite (101-|Am0). Physical Review B, 1997, 55, R16009-R16012.	3.2	28
74	Total-Reflection Inelastic X-Ray Scattering from a 10-nm Thick<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>La</mml:mi><mml:mn>0.6</mml:mn></mml:msub><mml:msub><mml:mi>Sr</mml:mi><mml:m Film. Physical Review Letters, 2011, 106, 037401.	7.8	27
75	Graphene-Supported Monometallic and Bimetallic Dimers for Electrochemical CO2 Reduction. Journal of Physical Chemistry C, 2018, 122, 28629-28636.	3.1	27
76	Coherent X-ray spectroscopy reveals the persistence of island arrangements during layer-by-layer growth. Nature Physics, 2019, 15, 589-594.	16.7	26
77	MoO_xS_y/Ni₃S₂ Microspheres on Ni Foam as Highly Efficient, Durable Electrocatalysts for Hydrogen Evolution Reaction. Chemistry of Materials, 2022, 34, 798-808.	6.7	26
78	Stable Subnanometer Cobalt Oxide Clusters on Ultrananocrystalline Diamond and Alumina Supports: Oxidation State and the Origin of Sintering Resistance. Journal of Physical Chemistry C, 2012, 116, 24027-24034.	3.1	24
79	Periodic ab initio calculations of orthoboric acid. Journal of Chemical Physics, 2000, 113, 3338-3343.	3.0	23
80	Increased reactivity of single wall carbon nanotubes at carbon ad-dimer defect sites. Chemical Physics Letters, 2007, 450, 71-75.	2.6	23
81	Highly Active Rhenium-, Ruthenium-, and Iridium-Based Dichalcogenide Electrocatalysts for Oxygen Reduction and Oxygen Evolution Reactions in Aprotic Media. Chemistry of Materials, 2020, 32, 2764-2773.	6.7	23
82	SIPs. ACM Transactions on Mathematical Software, 2007, 33, 9.	2.9	22
83	Nanostructured Conductive Metal Organic Frameworks for Sustainable Low Charge Overpotentials in Liâ€“Air Batteries. Small, 2022, 18, e2102902.	10.0	22
84	Excited State Dynamics and Structures of Functionalized Phthalocyanines. 1. Self-Regulated Assembly of Zinc Helicenocyanine. Journal of Physical Chemistry B, 2005, 109, 16598-16609.	2.6	21
85	Size-Selective Reactivity of Subnanometer Ag₄ and Ag₁₆ Clusters on a TiO₂ Surface. Journal of Physical Chemistry C, 2017, 121, 6614-6625.	3.1	21
86	Ca Cobaltites as Potential Cathode Materials for Rechargeable Ca-Ion Batteries: Theory and Experiment. Journal of Physical Chemistry C, 2020, 124, 5902-5909.	3.1	21
87	Atomic-Scale Study of Ambient-Pressure Redox-Induced Changes for an Oxide-Supported Submonolayer Catalyst: VO_x/Î±-TiO₂(110). Journal of Physical Chemistry Letters, 2012, 3, 2845-2850.	4.6	20
88	Water Oxidation Catalysis via Size-Selected Iridium Clusters. Journal of Physical Chemistry C, 2018, 122, 9965-9972.	3.1	20
89	Direct Observation of Electron Beam-Induced Phase Transition in MgCrMnO₄. Chemistry of Materials, 2020, 32, 10456-10462.	6.7	18
90	Theoretical analysis of hole self-trapping in ionic solids: Application to the KCl crystal. Physical Review B, 1993, 47, 14875-14885.	3.2	17

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91	Phonon and thermal transport properties of the misfit-layered oxide thermoelectric Ca3Co4O9 from first principles. Applied Physics Letters, 2014, 104, 251910.	3.3	17
92	On the variation of dissolution rates at the orthoclase (0 0 1) surface with pH and temperature. Geochimica Et Cosmochimica Acta, 2014, 141, 598-611.	3.9	16
93	Electronic and magnetic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">T</mml:mi><mml:msub><mml:mi mathvariant="normal">i</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>7</mml:mn></mml:msub></mml:mrow></mml:math>predicted by self-interaction-corrected density functional theory. Physical Review B, 2015, 91, .	3.2	16
94	Anomalous Kondo resonance mediated by semiconducting graphene nanoribbons in a molecular heterostructure. Nature Communications, 2017, 8, 946.	12.8	16
95	Investigation of Ca Insertion into Î±-MoO₃ Nanoparticles for High Capacity Ca-Ion Cathodes. Nano Letters, 2022, 22, 2228-2235.	9.1	16
96	Quantum chemical study of TiO2/dopamine-DNA triads. Chemical Physics, 2007, 339, 164-172.	1.9	15
97	First-Principles Study of Carbon and Vacancy Structures in Niobium. Journal of Physical Chemistry C, 2015, 119, 14728-14736.	3.1	15
98	Shiftâ€andâ€invert parallel spectral transformation eigensolver: Massively parallel performance for densityâ€functional based tightâ€binding. Journal of Computational Chemistry, 2016, 37, 448-459.	3.3	15
99	Kinetic Monte Carlo simulations of GaN homoepitaxy on c- and m-plane surfaces. Journal of Chemical Physics, 2017, 146, 144702.	3.0	15
100	Increasing Ionic Conductivity of Poly(ethylene oxide) by Reaction with Metallic Li. Advanced Energy and Sustainability Research, 2022, 3, 2100142.	5.8	15
101	Fabrication and characterization of platinum nanoparticle arrays of controlled size, shape and orientation. Electrochimica Acta, 2010, 55, 7934-7938.	5.2	14
102	Metallicity of InN and GaN surfaces exposed to NH3. Physical Review B, 2012, 85, .	3.2	14
103	Density functional study of the structure, thermodynamics and electronic properties of CdGeAs2. Journal of Physics Condensed Matter, 1999, 11, 4517-4526.	1.8	13
104	A DFT study of reaction pathways of NH3 decomposition on InN (0001) surface. Journal of Chemical Physics, 2012, 137, 054708.	3.0	13
105	Dynamic Field Modulation of the Octahedral Framework in Metal Oxide Heterostructures. Advanced Materials, 2018, 30, e1804775.	21.0	13
106	Theoretical Studies of CN and C₂ Addition to a (100)â€“(2 Ã— 1) Diamond Surface: Nanocrystalline Diamond Growth Mechanisms. Journal of Computational and Theoretical Nanoscience, 2005, 2, 207-213.	0.4	13
107	Density Functional Based Tight Binding Study of C2 and CN Deposition On (100) Diamond Surface. Materials Research Society Symposia Proceedings, 2001, 675, 1.	0.1	12
108	First-principles study of compensation mechanisms in negatively charged LaGaO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>/MgAl<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>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mml:	3.2	12

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109	Oxygen-modulated quantum conductance for ultrathin <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">HfO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> -based memristive switching devices. Physical Review B, 2016, 94, .	3.2	11
110	Real-time x-ray studies of crystal growth modes during metal-organic vapor phase epitaxy of GaN on c- and m-plane single crystals. Applied Physics Letters, 2014, 105, .	3.3	10
111	Atomic relaxation of the BeO (101Ì„0) surface. Surface Science, 1997, 381, L563-L567.	1.9	9
112	Theoretical study of the ionization potential of thymine: effect of adding conjugated functional groups. Chemical Physics Letters, 2003, 380, 54-62.	2.6	9
113	Self-consistent tight binding molecular dynamics study of TiO2 nanoclusters in water. Journal of Electroanalytical Chemistry, 2007, 607, 147-157.	3.8	9
114	Crystal Orientation-Dependent Reactivity of Oxide Surfaces in Contact with Lithium Metal. ACS Applied Materials & Interfaces, 2018, 10, 17471-17479.	8.0	9
115	Dissociative adsorption of hydrogen on the ZrB2(0001) surface. Surface Science, 2012, 606, 1808-1814.	1.9	8
116	Layered Transition Metal Oxides as Ca Intercalation Cathodes: A Systematic Firstâ€Principles Evaluation. Advanced Energy Materials, 2021, 11, 2101698.	19.5	8
117	Giant two-phonon Raman scattering from nanoscale NbC precipitates in Nb. Physical Review B, 2015, 91, .	3.2	7
118	SIESTAâ€SIPs: Massively parallel spectrumâ€slicing eigensolver for an ab initio molecular dynamics package. Journal of Computational Chemistry, 2018, 39, 1806-1814.	3.3	7
119	Quasicontinuum-Like Reduction of Density Functional Theory Calculations of Nanostructures. Journal of Nanoscience and Nanotechnology, 2008, 8, 3729-3740.	0.9	6
120	Dissociative adsorption of ammonia on the ZrB2(0001) surface. Surface Science, 2013, 615, 110-118.	1.9	6
121	Regioselective Oxidation of Strained Graphene for Controllable Synthesis of Nanoribbons. Journal of Physical Chemistry C, 2013, 117, 19160-19166.	3.1	6
122	In situ microbeam surface X-ray scattering reveals alternating step kinetics during crystal growth. Nature Communications, 2021, 12, 1721.	12.8	6
123	Designing silicon carbide heterostructures for quantum information science: challenges and opportunities. Materials for Quantum Technology, 2022, 2, 023001.	3.1	6
124	C₂adsorption on the (100) diamond surface: periodic and large cluster calculations. Molecular Physics, 2005, 103, 1017-1025.	1.7	5
125	Carbon nanotunnels form from single-walled carbon nanotubes interacting with a diamond (100)â€“(2Ã—1) surface. Diamond and Related Materials, 2011, 20, 1103-1109.	3.9	5
126	Dissociation of trimethylgallium on the ZrB2(0001) surface. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2013, 31, 061405.	2.1	5

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127	Fluorescence intermittency originates from reclustering in two-dimensional organic semiconductors. Nature Communications, 2017, 8, 14521.	12.8	5
128	Thermodynamic and kinetic properties of layered-CaCo₂O₄ for the Ca-ion batteries: a systematic first-principles study. Journal of Materials Chemistry A, 2020, 8, 21700-21710.	10.3	5
129	Island dynamics and anisotropy during vapor phase epitaxy of m-plane GaN. Applied Physics Letters, 2017, 111, .	3.3	5
130	Epitaxial oxide bilayer on Pt (001) nanofacets. Journal of Chemical Physics, 2012, 136, 044704.	3.0	4
131	Monitoring of dielectric permittivity in accelerated alkali-silica reaction concrete with microwave backscattering. Materials and Structures/Materiaux Et Constructions, 2020, 53, 1.	3.1	4
132	Effective diffusion coefficient and diffusion-controlled reactions in insulating solids with defects. Radiation Effects and Defects in Solids, 1995, 137, 295-297.	1.2	3
133	A note on the regularity of reduced models obtained by nonlocal quasi-continuum-like approaches. Mathematical Programming, 2009, 118, 207-236.	2.4	3
134	Electrocatalytic activity of surface oxides on platinum nanofacets and surfaces. Electrochimica Acta, 2013, 109, 440-446.	5.2	3
135	Structure and Reactivity of Molecularly Adsorbed Ammonia on the ZrB₂(0001) Surface. Journal of Physical Chemistry C, 2014, 118, 29260-29269.	3.1	3
136	An atomistic mechanism study of GaN step-flow growth in vicinal m-plane orientations. Physical Chemistry Chemical Physics, 2016, 18, 29239-29248.	2.8	3
137	Atomic-Scale Structure of Chemically Distinct Surface Oxygens in Redox Reactions. Journal of the American Chemical Society, 2021, 143, 17937-17941.	13.7	3
138	Theoretical investigation of the vibrational properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BeH</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Li</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub Physical Review B, 2009, 80, .	3.2	2
139	First-principles calculations of surfactant-assisted growth of polar CaO(111) oxide film: The case of water-based surfactant. Physical Review B, 2012, 86, .	3.2	2
140	Crystal truncation rods from miscut surfaces with alternating terminations. Physical Review B, 2021, 103, .	3.2	2
141	Simulating Nanoscale Processes in Solids Using DFT and the Quasicontinuum Method. , 2005, , .		2
142	Theoretical Studies of Growth Reactions on Diamond Surfaces. , 2004, , 266-307.		2
143	Theoretical investigation of the selfâ€trapped hole in alkali halides. I. Longâ€range effects within the model hamiltonian approach. Physica Status Solidi (B): Basic Research, 1994, 183, 201-221.	1.5	1
144	Theoretical Studies of UNCD Synthesis and Properties. , 2006, , 273-302.		1

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145	Theoretical Studies of UNCD Properties. , 2012, , 85-102.		1
146	Ab initio modeling of transport and thermodynamic stability for hafnia memristive devices. Journal of Computational Electronics, 2017, 16, 1066-1076.	2.5	1
147	Decomposition of ammonia on ZrB2(0001). Chemical Physics Letters, 2020, 739, 136984.	2.6	1
148	Theoretical evidence of water serving as a promoter for lithium superoxide disproportionation in Liâ€“O₂ batteries. Physical Chemistry Chemical Physics, 2021, 23, 10440-10447.	2.8	1
149	Burton-Cabrera-Frank theory for surfaces with alternating step types. Physical Review B, 2022, 105, .	3.2	1
150	First-Principles Study of Ï€-Bonded (100) Planar Defects in Diamond. Materials Research Society Symposia Proceedings, 1998, 538, 371.	0.1	0
151	Electronic Structure Studies of the Interaction of Water with a Cu(100) Surface. ACS Symposium Series, 2001, , 3-9.	0.5	0
152	Predicting the Energetics, Phase Stability, and Morphology Evolution of Faceted and Spherical Anatase Nanocrystals. ChemInform, 2005, 36, no.	0.0	0
153	Modeling Block Copolymer Interactions with Biomimetic Membranes. Materials Research Society Symposia Proceedings, 2006, 950, 1.	0.1	0
154	Explicit expressions for totally symmetric spherical functions and symmetry-dependent properties of multipoles. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2014, 470, 20140435.	2.1	0
155	A Real-Space Parallel Optimization Model Reduction Approach for Electronic Structure Computation in Large Nanostructures Using Orbital-Free Density Functional Theory. , 2006, , .		0