

Peter Zapol

List of Publications by Year in descending order

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155
papers

12,181
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157
all docs

157
docs citations

157
times ranked

15746
citing authors

#	ARTICLE	IF	CITATIONS
1	Increasing Ionic Conductivity of Poly(ethylene oxide) by Reaction with Metallic Li. Advanced Energy and Sustainability Research, 2022, 3, 2100142.	5.8	15
2	MoO _x S _y /Ni ₃ S ₂ Microspheres on Ni Foam as Highly Efficient, Durable Electrocatalysts for Hydrogen Evolution Reaction. Chemistry of Materials, 2022, 34, 798-808.	6.7	26
3	Burton-Cabrera-Frank theory for surfaces with alternating step types. Physical Review B, 2022, 105, .	3.2	1
4	Investigation of Ca Insertion into $\tilde{\pm}$ -MoO ₃ Nanoparticles for High Capacity Ca-Ion Cathodes. Nano Letters, 2022, 22, 2228-2235.	9.1	16
5	Nanostructured Conductive Metal Organic Frameworks for Sustainable Low Charge Overpotentials in Li ⁺ Air Batteries. Small, 2022, 18, e2102902.	10.0	22
6	Designing silicon carbide heterostructures for quantum information science: challenges and opportunities. Materials for Quantum Technology, 2022, 2, 023001.	3.1	6
7	Theoretical evidence of water serving as a promoter for lithium superoxide disproportionation in Li ⁺ O ₂ batteries. Physical Chemistry Chemical Physics, 2021, 23, 10440-10447.	2.8	1
8	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
9	2D Copper Tetrahydroxyquinone Conductive Metal-Organic Framework for Selective CO ₂ Electrocatalysis at Low Overpotentials. Advanced Materials, 2021, 33, e2004393.	21.0	120
10	In situ microbeam surface X-ray scattering reveals alternating step kinetics during crystal growth. Nature Communications, 2021, 12, 1721.	12.8	6
11	Crystal truncation rods from miscut surfaces with alternating terminations. Physical Review B, 2021, 103, .	3.2	2
12	Atomic-Scale Structure of Chemically Distinct Surface Oxygens in Redox Reactions. Journal of the American Chemical Society, 2021, 143, 17937-17941.	13.7	3
13	Layered Transition Metal Oxides as Ca Intercalation Cathodes: A Systematic First-Principles Evaluation. Advanced Energy Materials, 2021, 11, 2101698.	19.5	8
14	Probing Electrochemical Mg-Ion Activity in MgCr ₂ O ₄ Spinel Oxides. Chemistry of Materials, 2020, 32, 1162-1171.	6.7	31
15	Decomposition of ammonia on ZrB ₂ (0001). Chemical Physics Letters, 2020, 739, 136984.	2.6	1
16	Thermodynamic and kinetic properties of layered-CaCo ₂ O ₄ for the Ca-ion batteries: a systematic first-principles study. Journal of Materials Chemistry A, 2020, 8, 21700-21710.	10.3	5
17	High Voltage Mg-Ion Battery Cathode via a Solid Solution Cr _x Mn _{1-x} Spinel Oxide. Chemistry of Materials, 2020, 32, 6577-6587.	6.7	48
18	Direct Observation of Electron Beam-Induced Phase Transition in MgCrMnO ₄ . Chemistry of Materials, 2020, 32, 10456-10462.	6.7	18

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19	High Capacity for Mg ²⁺ Deintercalation in Spinel Vanadium Oxide Nanocrystals. <i>ACS Energy Letters</i> , 2020, 5, 2721-2727.	17.4	48
20	High-Voltage Phosphate Cathodes for Rechargeable Ca-Ion Batteries. <i>ACS Energy Letters</i> , 2020, 5, 3203-3211.	17.4	65
21	Monitoring of dielectric permittivity in accelerated alkali-silica reaction concrete with microwave backscattering. <i>Materials and Structures/Materiaux Et Constructions</i> , 2020, 53, 1.	3.1	4
22	Dynamic stability of active sites in hydr(oxy)oxides for the oxygen evolution reaction. <i>Nature Energy</i> , 2020, 5, 222-230.	39.5	540
23	Highly Active Rhenium-, Ruthenium-, and Iridium-Based Dichalcogenide Electrocatalysts for Oxygen Reduction and Oxygen Evolution Reactions in Aprotic Media. <i>Chemistry of Materials</i> , 2020, 32, 2764-2773.	6.7	23
24	Ca Cobaltites as Potential Cathode Materials for Rechargeable Ca-Ion Batteries: Theory and Experiment. <i>Journal of Physical Chemistry C</i> , 2020, 124, 5902-5909.	3.1	21
25	Highly Efficient Solar-Driven Carbon Dioxide Reduction on Molybdenum Disulfide Catalyst Using Choline Chloride-Based Electrolyte. <i>Advanced Energy Materials</i> , 2019, 9, 1803536.	19.5	34
26	Hierarchical Nanoassembly of MoS ₂ /Co ₉ S ₈ /Ni ₃ S ₂ /Ni as a Highly Efficient Electrocatalyst for Overall Water Splitting in a Wide pH Range. <i>Journal of the American Chemical Society</i> , 2019, 141, 10417-10430.	13.7	653
27	Coherent X-ray spectroscopy reveals the persistence of island arrangements during layer-by-layer growth. <i>Nature Physics</i> , 2019, 15, 589-594.	16.7	26
28	Dopant-Dependent Stability of Garnet Solid Electrolyte Interfaces with Lithium Metal. <i>Advanced Energy Materials</i> , 2019, 9, 1803440.	19.5	217
29	New Class of Electrocatalysts Based on 2D Transition Metal Dichalcogenides in Ionic Liquid. <i>Advanced Materials</i> , 2019, 31, e1804453.	21.0	43
30	Crystal Orientation-Dependent Reactivity of Oxide Surfaces in Contact with Lithium Metal. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 17471-17479.	8.0	9
31	Water Oxidation Catalysis via Size-Selected Iridium Clusters. <i>Journal of Physical Chemistry C</i> , 2018, 122, 9965-9972.	3.1	20
32	Graphene-Supported Monometallic and Bimetallic Dimers for Electrochemical CO ₂ Reduction. <i>Journal of Physical Chemistry C</i> , 2018, 122, 28629-28636.	3.1	27
33	Dynamic Field Modulation of the Octahedral Framework in Metal Oxide Heterostructures. <i>Advanced Materials</i> , 2018, 30, e1804775.	21.0	13
34	Vacancy-Mediated Anion Photosegregation Kinetics in Mixed Halide Hybrid Perovskites: Coupled Kinetic Monte Carlo and Optical Measurements. <i>ACS Energy Letters</i> , 2018, 3, 2321-2328.	17.4	119
35	SIESTA-SPPs: Massively parallel spectrum-slicing eigensolver for an <i>ab initio</i> molecular dynamics package. <i>Journal of Computational Chemistry</i> , 2018, 39, 1806-1814.	3.3	7
36	Three-dimensional imaging of dislocation dynamics during the hydriding phase transformation. <i>Nature Materials</i> , 2017, 16, 565-571.	27.5	81

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37	Revisiting the Corrosion of the Aluminum Current Collector in Lithium-Ion Batteries. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1072-1077.	4.6	156
38	Fluorescence intermittency originates from reclustering in two-dimensional organic semiconductors. <i>Nature Communications</i> , 2017, 8, 14521.	12.8	5
39	Copper Cluster Size Effect in Methanol Synthesis from CO ₂ . <i>Journal of Physical Chemistry C</i> , 2017, 121, 10406-10412.	3.1	144
40	Kinetic Monte Carlo simulations of GaN homoepitaxy on c- and m-plane surfaces. <i>Journal of Chemical Physics</i> , 2017, 146, 144702.	3.0	15
41	Size-Selective Reactivity of Subnanometer Ag ₄ and Ag ₁₆ Clusters on a TiO ₂ Surface. <i>Journal of Physical Chemistry C</i> , 2017, 121, 6614-6625.	3.1	21
42	Tailoring the Edge Structure of Molybdenum Disulfide toward Electrocatalytic Reduction of Carbon Dioxide. <i>ACS Nano</i> , 2017, 11, 453-460.	14.6	208
43	Anomalous Kondo resonance mediated by semiconducting graphene nanoribbons in a molecular heterostructure. <i>Nature Communications</i> , 2017, 8, 946.	12.8	16
44	Ab initio modeling of transport and thermodynamic stability for hafnia memristive devices. <i>Journal of Computational Electronics</i> , 2017, 16, 1066-1076.	2.5	1
45	Island dynamics and anisotropy during vapor phase epitaxy of m-plane GaN. <i>Applied Physics Letters</i> , 2017, 111, .	3.3	5
46	Shift-and-invert parallel spectral transformation eigensolver: Massively parallel performance for density-functional based tight-binding. <i>Journal of Computational Chemistry</i> , 2016, 37, 448-459.	3.3	15
47	An atomistic mechanism study of GaN step-flow growth in vicinal m-plane orientations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 29239-29248.	2.8	3
48	Nanostructured transition metal dichalcogenide electrocatalysts for CO ₂ reduction in ionic liquid. <i>Science</i> , 2016, 353, 467-470.	12.6	778
49	Interfacial control of oxygen vacancy doping and electrical conduction in thin film oxide heterostructures. <i>Nature Communications</i> , 2016, 7, 11892.	12.8	77
50	Oxygen-modulated quantum conductance for ultrathin HfO_2 -based memristive switching devices. <i>Physical Review B</i> , 2016, 94, .	3.2	11
51	Cathode Based on Molybdenum Disulfide Nanoflakes for Lithium-Oxygen Batteries. <i>ACS Nano</i> , 2016, 10, 2167-2175.	14.6	184
52	The effect of a Ta oxygen scavenger layer on HfO ₂ -based resistive switching behavior: thermodynamic stability, electronic structure, and low-bias transport. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 7502-7510.	2.8	31
53	Giant two-phonon Raman scattering from nanoscale NbC precipitates in Nb. <i>Physical Review B</i> , 2015, 91, .	3.2	7
54	Avalanching strain dynamics during the hydriding phase transformation in individual palladium nanoparticles. <i>Nature Communications</i> , 2015, 6, 10092.	12.8	87

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55	First-Principles Study of Carbon and Vacancy Structures in Niobium. <i>Journal of Physical Chemistry C</i> , 2015, 119, 14728-14736.	3.1	15
56	Carbon Dioxide Conversion to Methanol over Size-Selected Cu ₄ Clusters at Low Pressures. <i>Journal of the American Chemical Society</i> , 2015, 137, 8676-8679.	13.7	299
57	Electronic and magnetic properties of mml:math $\text{mathvariant} = \text{"normal"} > \text{T} < \text{mml:mi} < \text{mml:msub} < \text{mml:mi}$ $\text{mathvariant} = \text{"normal"} > \text{i} < \text{mml:mi} < \text{mml:mn} > 4 < \text{mml:mn} > < \text{mml:msub} < \text{mml:msub} < \text{mml:mi}$ $\text{mathvariant} = \text{"normal"} > \text{O} < \text{mml:mt} < \text{mml:mn} > 7 < \text{mml:mn} > < \text{mml:msub} < \text{mml:mrow} < \text{mml:math}$ predicted by self-interaction-corrected density functional theory. <i>Physical Review B</i> , 2015, 91, .	3.2	16
58	Structure and Reactivity of Molecularly Adsorbed Ammonia on the ZrB ₂ (0001) Surface. <i>Journal of Physical Chemistry C</i> , 2014, 118, 29260-29269.	3.1	3
59	Real-time x-ray studies of crystal growth modes during metal-organic vapor phase epitaxy of GaN on c- and m-plane single crystals. <i>Applied Physics Letters</i> , 2014, 105, .	3.3	10
60	Phonon and thermal transport properties of the misfit-layered oxide thermoelectric Ca ₃ Co ₄ O ₉ from first principles. <i>Applied Physics Letters</i> , 2014, 104, 251910.	3.3	17
61	Explicit expressions for totally symmetric spherical functions and symmetry-dependent properties of multipoles. <i>Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences</i> , 2014, 470, 20140435.	2.1	0
62	Computational studies of electrochemical CO ₂ reduction on subnanometer transition metal clusters. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26584-26599.	2.8	62
63	On the variation of dissolution rates at the orthoclase (0 0 1) surface with pH and temperature. <i>Geochimica Et Cosmochimica Acta</i> , 2014, 141, 598-611. First-principles study of compensation mechanisms in negatively charged LaGaO ₃ . mml:math $\text{xmlns:mml} = \text{"http://www.w3.org/1998/Math/MathML"} \text{ display} = \text{"inline"} > < \text{mml:msub} < \text{mml:mrow}$ $> < \text{mml:mn} > 3 < \text{mml:msub} < \text{mml:math} > \text{MgAl} < \text{mml:math}$	3.9	16
64	$\text{xmlns:mml} = \text{"http://www.w3.org/1998/Math/MathML"} \text{ display} = \text{"inline"} > < \text{mml:msub} < \text{mml:mrow}$ $> < \text{mml:mn} > 2 < \text{mml:msub} < \text{mml:math} > \text{O} < \text{mml:math}$ $\text{xmlns:mml} = \text{"http://www.w3.org/1998/Math/MathML"} \text{ display} = \text{"inline"} > < \text{mml:msub} < \text{mml:mrow}$ $> < \text{mml:math}$	3.2	12
65	Dissociative adsorption of ammonia on the ZrB ₂ (0001) surface. <i>Surface Science</i> , 2013, 615, 110-118.	1.9	6
66	Regioselective Oxidation of Strained Graphene for Controllable Synthesis of Nanoribbons. <i>Journal of Physical Chemistry C</i> , 2013, 117, 19160-19166.	3.1	6
67	Electrocatalytic activity of surface oxides on platinum nanofacets and surfaces. <i>Electrochimica Acta</i> , 2013, 109, 440-446.	5.2	3
68	First-principles Study of Hydrolysis Reaction Barriers in a Sodium Borosilicate Glass. <i>International Journal of Applied Glass Science</i> , 2013, 4, 395-407.	2.0	66
69	Dissociation of trimethylgallium on the ZrB ₂ (0001) surface. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2013, 31, 061405.	2.1	5
70	Epitaxial oxide bilayer on Pt (001) nanofacets. <i>Journal of Chemical Physics</i> , 2012, 136, 044704.	3.0	4
71	A DFT study of reaction pathways of NH ₃ decomposition on InN (0001) surface. <i>Journal of Chemical Physics</i> , 2012, 137, 054708.	3.0	13
72	First-principles calculations of surfactant-assisted growth of polar CaO(111) oxide film: The case of water-based surfactant. <i>Physical Review B</i> , 2012, 86, .	3.2	2

#	ARTICLE	Principles study of the atomic and electronic structures of misfit-layered calcium cobaltite	IF	CITATIONS
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#	ARTICLE	IF	CITATIONS
91	A Theoretical Study of CO ₂ Anions on Anatase (101) Surface. <i>Journal of Physical Chemistry C</i> , 2010, 114, 21474-21481.	3.1	159
92	A note on the regularity of reduced models obtained by nonlocal quasi-continuum-like approaches. <i>Mathematical Programming</i> , 2009, 118, 207-236.	2.4	3
93	Tailoring the Load Carrying Capacity of MWCNTs Through Inter-shell Atomic Bridging. <i>Experimental Mechanics</i> , 2009, 49, 169-182.	2.0	45
94	Subnanometre platinum clusters as highly active and selective catalysts for the oxidative dehydrogenation of propane. <i>Nature Materials</i> , 2009, 8, 213-216.	27.5	725
95	Monomeric Vanadium Oxide on a $\tilde{\gamma}$ -Al ₂ O ₃ Support: A Combined Experimental/Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 8836-8843.	3.1	52
96	Shape-Dependent Activity of Platinum Array Catalyst. <i>Journal of the American Chemical Society</i> , 2009, 131, 5732-5733.	13.7	134
97	Catalytic Fe-xN Sites in Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2009, 113, 21629-21634.	3.1	83
98	Theoretical investigation of the vibrational properties of BeH Li . <i>Physical Review B</i> , 2009, 80, .	3.2	msub
99	Measurements of near-ultimate strength for multiwalled carbon nanotubes and irradiation-induced crosslinking improvements. <i>Nature Nanotechnology</i> , 2008, 3, 626-631.	31.5	972
100	Quasicontinuum-Like Reduction of Density Functional Theory Calculations of Nanostructures. <i>Journal of Nanoscience and Nanotechnology</i> , 2008, 8, 3729-3740.	0.9	6
101	SIPs. <i>ACM Transactions on Mathematical Software</i> , 2007, 33, 9.	2.9	22
102	Order-disorder phase transition of the Cu(001) surface under equilibrium oxygen pressure. <i>Physical Review B</i> , 2007, 76, .	3.2	32
103	Shape of Platinum Nanoparticles Supported on SrTiO ₃ : Experiment and Theory. <i>Journal of Physical Chemistry C</i> , 2007, 111, 14782-14789.	3.1	42
104	Structure and Morphology of Hydroxylated Amorphous Alumina Surfaces. <i>Journal of Physical Chemistry C</i> , 2007, 111, 7422-7429.	3.1	53
105	Diffusion mechanisms of native point defects in rutile TiO ₂ :Ab initio total-energy calculations. <i>Physical Review B</i> , 2007, 75, .	3.2	107
106	Increased reactivity of single wall carbon nanotubes at carbon ad-dimer defect sites. <i>Chemical Physics Letters</i> , 2007, 450, 71-75.	2.6	23
107	Self-consistent tight binding molecular dynamics study of TiO ₂ nanoclusters in water. <i>Journal of Electroanalytical Chemistry</i> , 2007, 607, 147-157.	3.8	9
108	Quantum chemical study of TiO ₂ /dopamine-DNA triads. <i>Chemical Physics</i> , 2007, 339, 164-172.	1.9	15

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109	Quantum Chemical Study of Mechanisms for Oxidative Dehydrogenation of Propane on Vanadium Oxide. <i>Journal of Physical Chemistry B</i> , 2006, 110, 8363-8371.	2.6	54
110	Atomistic simulations of amorphous alumina surfaces. <i>Physical Review B</i> , 2006, 74, .	3.2	81
111	Modeling the structure and electronic properties of TiO ₂ nano particles. <i>Physical Review B</i> , 2006, 73, .	3.2	53
112	Theoretical Studies of UNCD Synthesis and Properties. , 2006, , 273-302.		1
113	Modeling Block Copolymer Interactions with Biomimetic Membranes. <i>Materials Research Society Symposia Proceedings</i> , 2006, 950, 1.	0.1	0
114	Transport properties of n-type ultrananocrystalline diamond films. <i>Physical Review B</i> , 2006, 74, .	3.2	40
115	Carbon Ad-Dimer Defects in Carbon Nanotubes. <i>Physical Review Letters</i> , 2006, 96, 075506.	7.8	70
116	A Real-Space Parallel Optimization Model Reduction Approach for Electronic Structure Computation in Large Nanostructures Using Orbital-Free Density Functional Theory. , 2006, , .		0
117	Density functional study of the TiO ₂ -dopamine complex. <i>Chemical Physics Letters</i> , 2005, 406, 306-311.	2.6	67
118	Shaping Nanometer-Scale Architecture Through Surface Chemistry. <i>Advanced Materials</i> , 2005, 17, 965-971.	21.0	125
119	Predicting the Energetics, Phase Stability, and Morphology Evolution of Faceted and Spherical Anatase Nanocrystals. <i>ChemInform</i> , 2005, 36, no.	0.0	0
120	Anatase and rutile surfaces with adsorbates representative of acidic and basic conditions. <i>Surface Science</i> , 2005, 582, 173-188.	1.9	107
121	C ₂ adsorption on the (100) diamond surface: periodic and large cluster calculations. <i>Molecular Physics</i> , 2005, 103, 1017-1025.	1.7	5
122	Excited State Dynamics and Structures of Functionalized Phthalocyanines. 1. Self-Regulated Assembly of Zinc Helicenocyanine. <i>Journal of Physical Chemistry B</i> , 2005, 109, 16598-16609.	2.6	21
123	Modeling the Morphology and Phase Stability of TiO ₂ Nanocrystals in Water. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 107-116.	5.3	191
124	Simulating Nanoscale Processes in Solids Using DFT and the Quasicontinuum Method. , 2005, , .		2
125	Theoretical Studies of CN and C ₂ Addition to a (100)-(2 Å- 1) Diamond Surface: Nanocrystalline Diamond Growth Mechanisms. <i>Journal of Computational and Theoretical Nanoscience</i> , 2005, 2, 207-213.	0.4	13
126	Charge Transfer Across the Nanocrystalline-DNA Interface: Probing DNA Recognition. <i>Nano Letters</i> , 2004, 4, 1017-1023.	9.1	164

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127	Predicting the Energetics, Phase Stability, and Morphology Evolution of Faceted and Spherical Anatase Nanocrystals. <i>Journal of Physical Chemistry B</i> , 2004, 108, 18435-18440.	2.6	115
128	A model for the phase stability of arbitrary nanoparticles as a function of size and shape. <i>Journal of Chemical Physics</i> , 2004, 121, 4276-4283.	3.0	253
129	Effects of particle morphology and surface hydrogenation on the phase stability of TiO ₂ . <i>Physical Review B</i> , 2004, 70, .	3.2	200
130	Theoretical Studies of Growth Reactions on Diamond Surfaces. , 2004, , 266-307.		2
131	Theoretical study of the ionization potential of thymine: effect of adding conjugated functional groups. <i>Chemical Physics Letters</i> , 2003, 380, 54-62.	2.6	9
132	Computational Studies of Catechol and Water Interactions with Titanium Oxide Nanoparticles. <i>Journal of Physical Chemistry B</i> , 2003, 107, 11419-11427.	2.6	208
133	Carbon dimers on the diamond (100) surface:â€¢,â€¢Growth and nucleation. <i>Physical Review B</i> , 2003, 68, .	3.2	52
134	Charge Distribution and Stability of Charged Carbon Nanotubes. <i>Physical Review Letters</i> , 2002, 89, 255503.	7.8	79
135	The effect of nitrogen addition to Ar/CH ₄ plasmas on the growth, morphology and field emission of ultrananocrystalline diamond. <i>Diamond and Related Materials</i> , 2002, 11, 43-48.	3.9	121
136	Lyotropic Liquid-Crystalline Gel Formation in a Room-Temperature Ionic Liquid. <i>Langmuir</i> , 2002, 18, 7258-7260.	3.5	229
137	Synthesis and characterization of highly-conducting nitrogen-doped ultrananocrystalline diamond films. <i>Applied Physics Letters</i> , 2001, 79, 1441-1443.	3.3	465
138	Tight-binding molecular-dynamics simulation of impurities in ultrananocrystalline diamond grain boundaries. <i>Physical Review B</i> , 2001, 65, .	3.2	267
139	Electronic Structure Studies of the Interaction of Water with a Cu(100) Surface. <i>ACS Symposium Series</i> , 2001, , 3-9.	0.5	0
140	Density Functional Based Tight Binding Study of C ₂ and CN Deposition On (100) Diamond Surface. <i>Materials Research Society Symposia Proceedings</i> , 2001, 675, 1.	0.1	12
141	Periodic ab initio calculations of orthoboric acid. <i>Journal of Chemical Physics</i> , 2000, 113, 3338-3343.	3.0	23
142	Assessment of Gaussian-3 and Density Functional Theories for Enthalpies of Formation of C ₁ â”“C ₁₆ Alkanes. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5850-5854.	2.5	231
143	Ab Initio and Density Functional Study of the Activation Barrier for Ethane Cracking in Cluster Models of Zeolite H-ZSM-5. <i>Journal of Physical Chemistry B</i> , 2000, 104, 1944-1949.	2.6	106
144	Density functional study of the structure, thermodynamics and electronic properties of CdGeAs ₂ . <i>Journal of Physics Condensed Matter</i> , 1999, 11, 4517-4526.	1.8	13

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145	Ab initio study of hydrogen adsorption on the ZnO (101̄,0) surface. <i>Surface Science</i> , 1999, 422, 1-7.	1.9	43
146	Theoretical Studies on Nanocrystalline Diamond: Nucleation by Dicarbon and Electronic Structure of Planar Defects. <i>Journal of Physical Chemistry B</i> , 1999, 103, 5459-5467.	2.6	58
147	First-Principles Study of C_2 -Bonded (100) Planar Defects in Diamond. <i>Materials Research Society Symposia Proceedings</i> , 1998, 538, 371.	0.1	0
148	Theoretical study of nonpolar surfaces of aluminum nitride: Zinc blende (110) and wurtzite (101-1 Am0). <i>Physical Review B</i> , 1997, 55, R16009-R16012.	3.2	28
149	An interatomic potential study of the properties of gallium nitride. <i>Journal of Physics Condensed Matter</i> , 1997, 9, 9517-9525.	1.8	65
150	Atomic relaxation of the BeO (101̄,0) surface. <i>Surface Science</i> , 1997, 381, L563-L567.	1.9	9
151	Atomistic calculations of defects in ZnGeP2. <i>Journal of Applied Physics</i> , 1996, 79, 671.	2.5	45
152	Ab initioprediction of GaN (101̄,0) and (110) anomalous surface relaxation. <i>Physical Review B</i> , 1996, 53, R4209-R4212.	3.2	56
153	Effective diffusion coefficient and diffusion-controlled reactions in insulating solids with defects. <i>Radiation Effects and Defects in Solids</i> , 1995, 137, 295-297.	1.2	3
154	Theoretical investigation of the self-trapped hole in alkali halides. I. Long-range effects within the model hamiltonian approach. <i>Physica Status Solidi (B): Basic Research</i> , 1994, 183, 201-221.	1.5	1
155	Theoretical analysis of hole self-trapping in ionic solids: Application to the KCl crystal. <i>Physical Review B</i> , 1993, 47, 14875-14885.	3.2	17