

# Peter Zapol

## List of Publications by Year in descending order

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155  
papers

12,181  
citations

34076

52  
h-index

25770

108  
g-index

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. <i>Advanced Energy and Sustainability Research</i> , 2022, 3, 2100142.	2.8	15
2	MoO <sub>3</sub> /Ni <sub>3</sub> S <sub>2</sub> Microspheres on Ni Foam as Highly Efficient, Durable Electrocatalysts for Hydrogen Evolution Reaction. <i>Chemistry of Materials</i> , 2022, 34, 798-808.	3.2	26
3	Burton-Cabrera-Frank theory for surfaces with alternating step types. <i>Physical Review B</i> , 2022, 105, .	1.1	1
4	Investigation of Ca Insertion into $\pm$ -MoO <sub>3</sub> Nanoparticles for High Capacity Ca-Ion Cathodes. <i>Nano Letters</i> , 2022, 22, 2228-2235.	4.5	16
5	Nanostructured Conductive Metal Organic Frameworks for Sustainable Low Charge Overpotentials in Li-Air Batteries. <i>Small</i> , 2022, 18, e2102902.	5.2	22
6	Designing silicon carbide heterostructures for quantum information science: challenges and opportunities. <i>Materials for Quantum Technology</i> , 2022, 2, 023001.	1.2	6
7	Theoretical evidence of water serving as a promoter for lithium superoxide disproportionation in Li-O <sub>2</sub> batteries. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 10440-10447.	1.3	1
8	Dynamically Stable Active Sites from Surface Evolution of Perovskite Materials during the Oxygen Evolution Reaction. <i>Journal of the American Chemical Society</i> , 2021, 143, 2741-2750.	6.6	156
9	2D Copper Tetrahydroxyquinone Conductive Metal-Organic Framework for Selective CO <sub>2</sub> Electro catalysis at Low Overpotentials. <i>Advanced Materials</i> , 2021, 33, e2004393.	11.1	120
10	In situ microbeam surface X-ray scattering reveals alternating step kinetics during crystal growth. <i>Nature Communications</i> , 2021, 12, 1721.	5.8	6
11	Crystal truncation rods from miscut surfaces with alternating terminations. <i>Physical Review B</i> , 2021, 103, .	1.1	2
12	Atomic-Scale Structure of Chemically Distinct Surface Oxygens in Redox Reactions. <i>Journal of the American Chemical Society</i> , 2021, 143, 17937-17941.	6.6	3
13	Layered Transition Metal Oxides as Ca Intercalation Cathodes: A Systematic First-Principles Evaluation. <i>Advanced Energy Materials</i> , 2021, 11, 2101698.	10.2	8
14	Probing Electrochemical Mg-Ion Activity in MgCr <sub>2</sub> V <sub>4</sub> O <sub>4</sub> Spinel Oxides. <i>Chemistry of Materials</i> , 2020, 32, 1162-1171.	3.2	31
15	Decomposition of ammonia on ZrB <sub>2</sub> (0001). <i>Chemical Physics Letters</i> , 2020, 739, 136984.	1.2	1
16	Thermodynamic and kinetic properties of layered-CaCo <sub>2</sub> O <sub>4</sub> for the Ca-ion batteries: a systematic first-principles study. <i>Journal of Materials Chemistry A</i> , 2020, 8, 21700-21710.	5.2	5
17	High Voltage Mg-Ion Battery Cathode via a Solid Solution Cr-Mn Spinel Oxide. <i>Chemistry of Materials</i> , 2020, 32, 6577-6587.	3.2	48
18	Direct Observation of Electron Beam-Induced Phase Transition in MgCrMnO <sub>4</sub> . <i>Chemistry of Materials</i> , 2020, 32, 10456-10462.	3.2	18

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19	High Capacity for Mg <sup>2+</sup> Deintercalation in Spinel Vanadium Oxide Nanocrystals. ACS Energy Letters, 2020, 5, 2721-2727.	8.8	48
20	High-Voltage Phosphate Cathodes for Rechargeable Ca-Ion Batteries. ACS Energy Letters, 2020, 5, 3203-3211.	8.8	65
21	Monitoring of dielectric permittivity in accelerated alkali-silica reaction concrete with microwave backscattering. Materials and Structures/Materiaux Et Constructions, 2020, 53, 1.	1.3	4
22	Dynamic stability of active sites in hydr(oxy)oxides for the oxygen evolution reaction. Nature Energy, 2020, 5, 222-230.	19.8	540
23	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.	3.2	23
24	Ca Cobaltites as Potential Cathode Materials for Rechargeable Ca-Ion Batteries: Theory and Experiment. Journal of Physical Chemistry C, 2020, 124, 5902-5909.	1.5	21
25	Highly Efficient Solar-Driven Carbon Dioxide Reduction on Molybdenum Disulfide Catalyst Using Choline Chloride-Based Electrolyte. Advanced Energy Materials, 2019, 9, 1803536.	10.2	34
26	Hierarchical Nanoassembly of MoS <sub>2</sub> /Co <sub>9</sub> S <sub>8</sub> /Ni <sub>3</sub> S <sub>2</sub> /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.	6.6	653
27	Coherent X-ray spectroscopy reveals the persistence of island arrangements during layer-by-layer growth. Nature Physics, 2019, 15, 589-594.	6.5	26
28	Dopant-Dependent Stability of Garnet Solid Electrolyte Interfaces with Lithium Metal. Advanced Energy Materials, 2019, 9, 1803440.	10.2	217
29	New Class of Electrocatalysts Based on 2D Transition Metal Dichalcogenides in Ionic Liquid. Advanced Materials, 2019, 31, e1804453.	11.1	43
30	Crystal Orientation-Dependent Reactivity of Oxide Surfaces in Contact with Lithium Metal. ACS Applied Materials & Interfaces, 2018, 10, 17471-17479.	4.0	9
31	Water Oxidation Catalysis via Size-Selected Iridium Clusters. Journal of Physical Chemistry C, 2018, 122, 9965-9972.	1.5	20
32	Graphene-Supported Monometallic and Bimetallic Dimers for Electrochemical CO <sub>2</sub> Reduction. Journal of Physical Chemistry C, 2018, 122, 28629-28636.	1.5	27
33	Dynamic Field Modulation of the Octahedral Framework in Metal Oxide Heterostructures. Advanced Materials, 2018, 30, e1804775.	11.1	13
34	Vacancy-Mediated Anion Photo-segregation Kinetics in Mixed Halide Hybrid Perovskites: Coupled Kinetic Monte Carlo and Optical Measurements. ACS Energy Letters, 2018, 3, 2321-2328.	8.8	119
35	SIESTA-ESIPs: Massively parallel spectrum-slicing eigensolver for an <i>ab initio</i> molecular dynamics package. Journal of Computational Chemistry, 2018, 39, 1806-1814.	1.5	7
36	Three-dimensional imaging of dislocation dynamics during the hydriding phase transformation. Nature Materials, 2017, 16, 565-571.	13.3	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.	2.1	156
38	Fluorescence intermittency originates from reclustered in two-dimensional organic semiconductors. <i>Nature Communications</i> , 2017, 8, 14521.	5.8	5
39	Copper Cluster Size Effect in Methanol Synthesis from CO <sub>2</sub> . <i>Journal of Physical Chemistry C</i> , 2017, 121, 10406-10412.	1.5	144
40	Kinetic Monte Carlo simulations of GaN homoepitaxy on c- and m-plane surfaces. <i>Journal of Chemical Physics</i> , 2017, 146, 144702.	1.2	15
41	Size-Selective Reactivity of Subnanometer Ag <sub>4</sub> and Ag <sub>16</sub> Clusters on a TiO <sub>2</sub> Surface. <i>Journal of Physical Chemistry C</i> , 2017, 121, 6614-6625.	1.5	21
42	Tailoring the Edge Structure of Molybdenum Disulfide toward Electrocatalytic Reduction of Carbon Dioxide. <i>ACS Nano</i> , 2017, 11, 453-460.	7.3	208
43	Anomalous Kondo resonance mediated by semiconducting graphene nanoribbons in a molecular heterostructure. <i>Nature Communications</i> , 2017, 8, 946.	5.8	16
44	Ab initio modeling of transport and thermodynamic stability for hafnia memristive devices. <i>Journal of Computational Electronics</i> , 2017, 16, 1066-1076.	1.3	1
45	Island dynamics and anisotropy during vapor phase epitaxy of m-plane GaN. <i>Applied Physics Letters</i> , 2017, 111, .	1.5	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.	1.5	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.	1.3	3
48	Nanostructured transition metal dichalcogenide electrocatalysts for CO <sub>2</sub> reduction in ionic liquid. <i>Science</i> , 2016, 353, 467-470.	6.0	778
49	Interfacial control of oxygen vacancy doping and electrical conduction in thin film oxide heterostructures. <i>Nature Communications</i> , 2016, 7, 11892.	5.8	77
50	Oxygen-modulated quantum conductance for ultrathin HfO <sub>2</sub> -based memristive switching devices. <i>Physical Review B</i> , 2016, 94, .	1.1	11
51	Cathode Based on Molybdenum Disulfide Nanoflakes for Lithium-Oxygen Batteries. <i>ACS Nano</i> , 2016, 10, 2167-2175.	7.3	184
52	The effect of a Ta oxygen scavenger layer on HfO <sub>2</sub> -based resistive switching behavior: thermodynamic stability, electronic structure, and low-bias transport. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 7502-7510.	1.3	31
53	Giant two-phonon Raman scattering from nanoscale NbC precipitates in Nb. <i>Physical Review B</i> , 2015, 91, .	1.1	7
54	Avalanching strain dynamics during the hydriding phase transformation in individual palladium nanoparticles. <i>Nature Communications</i> , 2015, 6, 10092.	5.8	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.	1.5	15
56	Carbon Dioxide Conversion to Methanol over Size-Selected Cu <sub>4</sub> Clusters at Low Pressures. <i>Journal of the American Chemical Society</i> , 2015, 137, 8676-8679. <i>Electronic and magnetic properties of</i>	6.6	299
57	$T_i O_7$ predicted by self-interaction-corrected density functional theory. <i>Physical Review B</i> , 2015, 91.	1.1	16
58	Structure and Reactivity of Molecularly Adsorbed Ammonia on the ZrB <sub>2</sub> (0001) Surface. <i>Journal of Physical Chemistry C</i> , 2014, 118, 29260-29269.	1.5	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, .	1.5	10
60	Phonon and thermal transport properties of the misfit-layered oxide thermoelectric Ca <sub>3</sub> Co <sub>4</sub> O <sub>9</sub> from first principles. <i>Applied Physics Letters</i> , 2014, 104, 251910.	1.5	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.	1.0	0
62	Computational studies of electrochemical CO <sub>2</sub> reduction on subnanometer transition metal clusters. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26584-26599.	1.3	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 <sub>3</sub>	1.6	16
64	$MgAl_2O_4$	1.1	12
65	Dissociative adsorption of ammonia on the ZrB <sub>2</sub> (0001) surface. <i>Surface Science</i> , 2013, 615, 110-118.	0.8	6
66	Regioselective Oxidation of Strained Graphene for Controllable Synthesis of Nanoribbons. <i>Journal of Physical Chemistry C</i> , 2013, 117, 19160-19166.	1.5	6
67	Electrocatalytic activity of surface oxides on platinum nanofacets and surfaces. <i>Electrochimica Acta</i> , 2013, 109, 440-446.	2.6	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.	1.0	66
69	Dissociation of trimethylgallium on the ZrB <sub>2</sub> (0001) surface. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2013, 31, 061405.	0.9	5
70	Epitaxial oxide bilayer on Pt (001) nanofacets. <i>Journal of Chemical Physics</i> , 2012, 136, 044704.	1.2	4
71	A DFT study of reaction pathways of NH <sub>3</sub> decomposition on InN (0001) surface. <i>Journal of Chemical Physics</i> , 2012, 137, 054708.	1.2	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, .	1.1	2

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73	inciples study of the atomic and electronic structures of misfit-layered calcium cobaltite		
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91	A Theoretical Study of CO <sub>2</sub> Anions on Anatase (101) Surface. Journal of Physical Chemistry C, 2010, 114, 21474-21481.	1.5	159
92	A note on the regularity of reduced models obtained by nonlocal quasi-continuum-like approaches. Mathematical Programming, 2009, 118, 207-236.	1.6	3
93	Tailoring the Load Carrying Capacity of MWCNTs Through Inter-shell Atomic Bridging. Experimental Mechanics, 2009, 49, 169-182.	1.1	45
94	Subnanometre platinum clusters as highly active and selective catalysts for the oxidative dehydrogenation of propane. Nature Materials, 2009, 8, 213-216.	13.3	725
95	Monomeric Vanadium Oxide on a $\gamma$ -Al <sub>2</sub> O <sub>3</sub> Support: A Combined Experimental/Theoretical Study. Journal of Physical Chemistry C, 2009, 113, 8836-8843.	1.5	52
96	Shape-Dependent Activity of Platinum Array Catalyst. Journal of the American Chemical Society, 2009, 131, 5732-5733.	6.6	134
97	Catalytic Fe-xN Sites in Carbon Nanotubes. Journal of Physical Chemistry C, 2009, 113, 21629-21634.	1.5	83
98	Theoretical investigation of the vibrational properties of $\text{BeH}_2$ $\text{Li}_2$ Physical Review B, 2009, 80, .	1.1	2
99	Measurements of near-ultimate strength for multiwalled carbon nanotubes and irradiation-induced crosslinking improvements. Nature Nanotechnology, 2008, 3, 626-631.	15.6	972
100	Quasicontinuum-Like Reduction of Density Functional Theory Calculations of Nanostructures. Journal of Nanoscience and Nanotechnology, 2008, 8, 3729-3740.	0.9	6
101	SIPs. ACM Transactions on Mathematical Software, 2007, 33, 9.	1.6	22
102	Order-disorder phase transition of the Cu(001) surface under equilibrium oxygen pressure. Physical Review B, 2007, 76, .	1.1	32
103	Shape of Platinum Nanoparticles Supported on SrTiO <sub>3</sub> : $\delta$ Experiment and Theory. Journal of Physical Chemistry C, 2007, 111, 14782-14789.	1.5	42
104	Structure and Morphology of Hydroxylated Amorphous Alumina Surfaces. Journal of Physical Chemistry C, 2007, 111, 7422-7429.	1.5	53
105	Diffusion mechanisms of native point defects in rutile TiO <sub>2</sub> : Ab initio total-energy calculations. Physical Review B, 2007, 75, .	1.1	107
106	Increased reactivity of single wall carbon nanotubes at carbon ad-dimer defect sites. Chemical Physics Letters, 2007, 450, 71-75.	1.2	23
107	Self-consistent tight binding molecular dynamics study of TiO <sub>2</sub> nanoclusters in water. Journal of Electroanalytical Chemistry, 2007, 607, 147-157.	1.9	9
108	Quantum chemical study of TiO <sub>2</sub> /dopamine-DNA triads. Chemical Physics, 2007, 339, 164-172.	0.9	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.	1.2	54
110	Atomistic simulations of amorphous alumina surfaces. <i>Physical Review B</i> , 2006, 74, .	1.1	81
111	Modeling the structure and electronic properties of TiO <sub>2</sub> nanoparticles. <i>Physical Review B</i> , 2006, 73, .	1.1	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, .	1.1	40
115	Carbon Ad-Dimer Defects in Carbon Nanotubes. <i>Physical Review Letters</i> , 2006, 96, 075506.	2.9	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 <sub>2</sub> –dopamine complex. <i>Chemical Physics Letters</i> , 2005, 406, 306-311.	1.2	67
118	Shaping Nanometer-Scale Architecture Through Surface Chemistry. <i>Advanced Materials</i> , 2005, 17, 965-971.	11.1	125
119	Predicting the Energetics, Phase Stability, and Morphology Evolution of Faceted and Spherical Anatase Nanocrystals. <i>ChemInform</i> , 2005, 36, no.	0.1	0
120	Anatase and rutile surfaces with adsorbates representative of acidic and basic conditions. <i>Surface Science</i> , 2005, 582, 173-188.	0.8	107
121	C <sub>2</sub> adsorption on the (100) diamond surface: periodic and large cluster calculations. <i>Molecular Physics</i> , 2005, 103, 1017-1025.	0.8	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.	1.2	21
123	Modeling the Morphology and Phase Stability of TiO <sub>2</sub> Nanocrystals in Water. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 107-116.	2.3	191
124	Simulating Nanoscale Processes in Solids Using DFT and the Quasicontinuum Method. , 2005, , .		2
125	Theoretical Studies of CN and C <sub>2</sub> 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.	4.5	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.	1.2	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.	1.2	253
129	Effects of particle morphology and surface hydrogenation on the phase stability of TiO <sub>2</sub> . <i>Physical Review B</i> , 2004, 70, .	1.1	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.	1.2	9
132	Computational Studies of Catechol and Water Interactions with Titanium Oxide Nanoparticles. <i>Journal of Physical Chemistry B</i> , 2003, 107, 11419-11427.	1.2	208
133	Carbon dimers on the diamond (100) surface: Growth and nucleation. <i>Physical Review B</i> , 2003, 68, .	1.1	52
134	Charge Distribution and Stability of Charged Carbon Nanotubes. <i>Physical Review Letters</i> , 2002, 89, 255503.	2.9	79
135	The effect of nitrogen addition to Ar/CH <sub>4</sub> plasmas on the growth, morphology and field emission of ultrananocrystalline diamond. <i>Diamond and Related Materials</i> , 2002, 11, 43-48.	1.8	121
136	Lyotropic Liquid-Crystalline Gel Formation in a Room-Temperature Ionic Liquid. <i>Langmuir</i> , 2002, 18, 7258-7260.	1.6	229
137	Synthesis and characterization of highly-conducting nitrogen-doped ultrananocrystalline diamond films. <i>Applied Physics Letters</i> , 2001, 79, 1441-1443.	1.5	465
138	Tight-binding molecular-dynamics simulation of impurities in ultrananocrystalline diamond grain boundaries. <i>Physical Review B</i> , 2001, 65, .	1.1	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 <sub>2</sub> 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.	1.2	23
142	Assessment of Gaussian-3 and Density Functional Theories for Enthalpies of Formation of C <sub>1</sub> ~C <sub>16</sub> Alkanes. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5850-5854.	1.1	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.	1.2	106
144	Density functional study of the structure, thermodynamics and electronic properties of CdGeAs <sub>2</sub> . <i>Journal of Physics Condensed Matter</i> , 1999, 11, 4517-4526.	0.7	13

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145	Ab initio study of hydrogen adsorption on the ZnO (101̄,0) surface. Surface Science, 1999, 422, 1-7.	0.8	43
146	Theoretical Studies on Nanocrystalline Diamond: Nucleation by Dicarbon and Electronic Structure of Planar Defects. Journal of Physical Chemistry B, 1999, 103, 5459-5467.	1.2	58
147	First-Principles Study of Ĩ-Bonded (100) Planar Defects in Diamond. Materials Research Society Symposia Proceedings, 1998, 538, 371.	0.1	0
148	Theoretical study of nonpolar surfaces of aluminum nitride: Zinc blende (110) and wurtzite (101- Am0). Physical Review B, 1997, 55, R16009-R16012.	1.1	28
149	An interatomic potential study of the properties of gallium nitride. Journal of Physics Condensed Matter, 1997, 9, 9517-9525.	0.7	65
150	Atomic relaxation of the BeO (101̄,0) surface. Surface Science, 1997, 381, L563-L567.	0.8	9
151	Atomistic calculations of defects in ZnGeP2. Journal of Applied Physics, 1996, 79, 671.	1.1	45
152	Ab initio prediction of GaN (101̄0) and (110) anomalous surface relaxation. Physical Review B, 1996, 53, R4209-R4212.	1.1	56
153	Effective diffusion coefficient and diffusion-controlled reactions in insulating solids with defects. Radiation Effects and Defects in Solids, 1995, 137, 295-297.	0.4	3
154	Theoretical investigation of the self-trapped hole in alkali halides. I. Long-range effects within the model hamiltonian approach. Physica Status Solidi (B): Basic Research, 1994, 183, 201-221.	0.7	1
155	Theoretical analysis of hole self-trapping in ionic solids: Application to the KCl crystal. Physical Review B, 1993, 47, 14875-14885.	1.1	17