Hiroshi Mizuseki

List of Publications by Year
in descending order

267	6,032	87843 38	114418 63
papers	citations	h-index	g-index

267	267	267	6706
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A theoretical study on the interaction of aromatic amino acids with graphene and single walled carbon nanotube. Journal of Chemical Physics, 2009, 130, 124911.	1.2	251
2	Machine-Learning-Assisted Accurate Band Gap Predictions of Functionalized MXene. Chemistry of Materials, 2018, 30, 4031-4038.	3.2	235
3	Mechanistic Insight into the Chemical Exfoliation and Functionalization of Ti₃C₂ MXene. ACS Applied Materials & Interfaces, 2016, 8, 24256-24264.	4.0	221
4	Designing Nanogadgetry for Nanoelectronic Devices with Nitrogenâ€Doped Capped Carbon Nanotubes. Small, 2009, 5, 1769-1775.	5.2	176
5	Electronic structure and optical properties of the Co-doped anataseTiO2studied from first principles. Physical Review B, 2004, 69, .	1.1	161
6	Influence of Molecular Geometry, Exchange-Correlation Functional, and Solvent Effects in the Modeling of Vertical Excitation Energies in Phthalocyanines Using Time-Dependent Density Functional Theory (TDDFT) and Polarized Continuum Model TDDFT Methods:â€‰ Can Modern Computational Chemistry Methods Explain Experimental Controversies?. Journal of Physical Chemistry A, 2007, 111, 12901-12913.	1.1	149
7	Band Structures of Perovskite-Like Fluorides for Vacuum-Ultraviolet-Transparent Lens Materials. Japanese Journal of Applied Physics, 2002, 41, L365-L367.	0.8	132
8	Tuning the Electronic and Magnetic Properties of Phosphorene by Vacancies and Adatoms. Journal of Physical Chemistry C, 2015, 119, 6530-6538.	1.5	125
9	Vacancy induced structural and magnetic transition in MnCo1â^'xGe. Applied Physics Letters, 2006, 89, 262504.	1.5	121
10	Electronic transport through bent carbon nanotubes: Nanoelectromechanical sensors and switches. Physical Review B, 2003, 67, .	1.1	114
11	Cesium encapsulation in single-walled carbon nanotubes via plasma ion irradiation: Application to junction formation andab initioinvestigation. Physical Review B, 2003, 68, .	1.1	102
12	Engineering of Band Gap in Metalâ€“Organic Frameworks by Functionalizing Organic Linker: A Systematic Density Functional Theory Investigation. Journal of Physical Chemistry C, 2014, 118, 4567-4577.	1.5	97
13	Tetrahexcarbon: A two-dimensional allotrope of carbon. Carbon, 2018, 137, 266-273.	5.4	91
14	First-principles study of hydrogen storage over Ni and Rh doped BN sheets. Chemical Physics, 2009, 359, 173-178.	0.9	84
15	Energetics and local spin magnetic moment of single3,4dimpurities encapsulated in an icosahedralAu12cage. Physical Review B, 2004, 70, .	1.1	69
16	Modular, Homochiral, Porous Coordination Polymers: Rational Design, Enantioselective Guest Exchange Sorption and Ab Initio Calculations of Hostâ€“Guest Interactions. Chemistry - A European Journal, 2010, 16, 10348-10356.	1.7	67
17	C568: A new two-dimensional sp2-sp3 hybridized allotrope of carbon. Carbon, 2020, 158, 827-835.	5.4	62
18	Structural investigation of thiophene thiol adsorption on Au nanoclusters: Influence of back bonds. Journal of Chemical Physics, 2002, 117, 2819-2822.	1.2	58

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19	Theoretical insights into the formation, structure, and electronic properties of anticancer oxaliplatin drug and cucurbit[n]urils nÂ=Â5 to 8. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2010, 66, 213-218.	1.6	54
20	Titanium-Doped Nickel Clusters TiNin (n = 1â˜12): Geometry, Electronic, Magnetic, and Hydrogen Adsorption Properties. Journal of Physical Chemistry A, 2010, 114, 5049-5057.	1.1	53
21	First-principles study of the electronic structures of icosahedral TiNâ€Š(N=13,19,43,55) clusters. Journal of Chemical Physics, 2004, 120, 8463-8468.	1.2	49
22	Orthorhombic carbon oC24: A novel topological nodal line semimetal. Carbon, 2018, 133, 39-43.	5.4	48
23	Isolation of pristine MXene from Nb₄AlC₃ MAX phase: a first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 11073-11080.	1.3	47
24	Molecular Scale Rectifier:Â Theoretical Study. Journal of Physical Chemistry A, 2001, 105, 9454-9459.	1.1	45
25	Proposed design principle of fluoride-based materials for deep ultraviolet light emitting devices. Optical Materials, 2007, 30, 15-17.	1.7	45
26	Accurate description of phase diagram of clathrate hydrates at the molecular level. Journal of Chemical Physics, 2009, 131, 244510.	1.2	44
27	First-principles study of structural stability, magnetism, and hyperfine coupling in hydrogen clusters adsorbed on graphene. Physical Review B, 2010, 82, .	1.1	44
28	Kinetic Origin of Divergent Decompression Pathways in Silicon and Germanium. Physical Review Letters, 2013, 110, 165503.	2.9	44
29	Atomistic Origin of Phase Stability in Oxygen-Functionalized MXene: A Comparative Study. Journal of Physical Chemistry C, 2017, 121, 18947-18953.	1.5	44
30	Theoretical study of phase transitions in Kr and Ar clathrate hydrates from structure II to structure I under pressure. Journal of Chemical Physics, 2009, 131, 114507.	1.2	43
31	Accelerated Data-Driven Accurate Positioning of the Band Edges of MXenes. Journal of Physical Chemistry Letters, 2019, 10, 780-785.	2.1	43
32	Theoretical Prediction of the Complexation Behaviors of Antitumor Platinum Drugs with Cucurbiturils. Journal of Physical Chemistry B, 2012, 116, 14029-14039.	1.2	42
33	Control of substituent ligand over current through molecular devices: Anab initiomolecular orbital theory. Physical Review B, 2003, 67, .	1.1	41
34	Hydrogen storage capacity of C60(OM)12 (M=Li and Na) clusters. Journal of Chemical Physics, 2009, 131, 214505.	1.2	41
35	Atomic and electronic structures of neutral and cationSnn(n=2â€“20)clusters: A comparative theoretical study with different exchange-correlation functionals. Physical Review B, 2005, 71, .	1.1	40
36	Chemical engineering of prehydrogenated C and BN-sheets by Li: Application in hydrogen storage. Journal of Applied Physics, 2009, 106, .	1.1	40

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37	Theoretical investigation on the alkali-metal doped BN fullerene as a material for hydrogen storage. Chemical Physics, 2010, 377, 54-59.	0.9	39
38	Strong chromate-adsorbent based on pyrrolic nitrogen structure: An experimental and theoretical study on the adsorption mechanism. Water Research, 2018, 145, 287-296.	5.3	39
39	Interactions of a conjugated molecular diode with small metal clusters of Cu, Ag, and Au: First-principles calculations. Journal of Chemical Physics, 2002, 117, 7669-7675.	1.2	38
40	Terahertz phonon modes of an intermolecular network of hydrogen bonds in an anhydrous Î²-d-glucopyranose crystal. Chemical Physics Letters, 2006, 423, 439-444.	1.2	38
41	The role of Li and Ni metals in the adsorbate complex and their effect on the hydrogen storage capacity of single walled carbon nanotubes coated with metal hydrides, LiH and NiH2. International Journal of Hydrogen Energy, 2010, 35, 2368-2376.	3.8	38
42	Improved Stability and Catalytic Properties of Au16 Cluster Supported on Graphane. Journal of Physical Chemistry C, 2011, 115, 20168-20174.	1.5	38
43	Encapsulation of cesium inside single-walled carbon nanotubes by plasma-ion irradiation method. Thin Solid Films, 2003, 435, 307-311.	0.8	37
44	Tuning Electronic Structure of Graphene: A First-Principles Study. IEEE Nanotechnology Magazine, 2012, 11, 534-541.	1.1	37
45	First-principles study of phenyl ethylene oligomers as current-switch. Physics Letters, Section A: General, Atomic and Solid State Physics, 2006, 359, 487-493.	0.9	35
46	THEORETICAL STUDY OF DONORâ€“SPACERâ€“ACCEPTOR STRUCTURE MOLECULE FOR STABLE MOLECULAR RECTIFIER. Molecular Crystals and Liquid Crystals, 2003, 406, 11-17.	0.4	34
47	First-principles study of intrinsic defect properties in hexagonal BN bilayer and monolayer. Solid State Communications, 2012, 152, 816-820.	0.9	34
48	Theoretical study of phthalocyanineâ€“fullerene complex for a high efficiency photovoltaic device using ab initio electronic structure calculation. Synthetic Metals, 2003, 138, 281-283.	2.1	33
49	Calcium-decorated graphene for hydrogen storage: A van der Waals density functional study. Computational Materials Science, 2012, 55, 180-185.	1.4	33
50	Band gap engineering of silicene zigzag nanoribbons with perpendicular electric fields: a theoretical study. Journal of Physics Condensed Matter, 2012, 24, 455302.	0.7	33
51	New carbon allotropes in sp + sp³ bonding networks consisting of C₈ cubes. Physical Chemistry Chemical Physics, 2018, 20, 7962-7967.	1.3	33
52	Direct numerical simulation of oscillatory Marangoni convection in cylindrical liquid bridges. Journal of Crystal Growth, 1999, 204, 395-404.	0.7	32
53	A general-purpose approach for calculating transport in contactâ€“moleculeâ€“contact systems: TARABORD implementation and application to a polythiophene-based nanodevice. Thin Solid Films, 2006, 499, 269-274.	0.8	31
54	Phase stability of carbon clathrates at high pressure. Journal of Applied Physics, 2010, 107, .	1.1	31

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55	The medium- and short-range collective atomic motion in Pdî—¸Si(Ge) amorphous alloys. Journal of Non-Crystalline Solids, 1993, 156-158, 58-62.	1.5	30
56	Quantum length dependence of conductance in oligomers: First-principles calculations. Physical Review B, 2007, 75, .	1.1	30
57	First-principles study of length dependence of conductance in alkanedithiols. Journal of Chemical Physics, 2008, 128, 044704.	1.2	30
58	Theoretical Study on Inclusion Complex of Polyaniline Covered by Cyclodextrins for Molecular Device. Japanese Journal of Applied Physics, 2002, 41, 2739-2741.	0.8	29
59	Fragmentation of small tin cluster ions (Snx+: x=4â€“20) in the low-energy collisions with a highly oriented pyrolytic graphite surface. Journal of Chemical Physics, 2002, 117, 4317-4322.	1.2	29
60	Three-Dimensional Carbon Allotropes Comprising Phenyl Rings and Acetylenic Chains in sp+sp2 Hybrid Networks. Scientific Reports, 2016, 6, 24665.	1.6	29
61	Design of wide-gap fluoride heterostructures for deep ultraviolet optical devices. Journal of Applied Physics, 2004, 96, 7655-7659.	1.1	28
62	Three-dimensional oscillatory convection of LiCaAlF6 melts in Czochralski crystal growth. Journal of Crystal Growth, 2003, 252, 538-549.	0.7	27
63	Hydrogen Adsorption on Lithium-Functionalized Calixarenes: A Computational Study. Journal of Physical Chemistry C, 2008, 112, 19676-19679.	1.5	27
64	Stability and Composition of Helium Hydrates Based on Ices I_h and II at Low Temperatures. Journal of Physical Chemistry C, 2014, 118, 2587-2593.	1.5	27
65	Marangoni convection in model of floating zone under microgravity. Journal of Crystal Growth, 2001, 229, 601-604.	0.7	26
66	The Role of Aromaticity and the Ï€â€Conjugated Framework in Multiporphyrinic Systems as Singleâ€Molecule Switches. Small, 2008, 4, 962-969.	5.2	26
67	Probing the Structure, Stability and Hydrogen Adsorption of Lithium Functionalized Isoreticular MOF-5 (Fe, Cu, Co, Ni and Zn) by Density Functional Theory. International Journal of Molecular Sciences, 2009, 10, 1601-1608.	1.8	26
68	Geometrical indications of adsorbed hydrogen atoms on graphite producing star and ellipsoidal like features in scanning tunneling microscopy images: Ab initio study. Carbon, 2009, 47, 3306-3312.	5.4	26
69	Electronic structures and spectra of symmetric mesoâ€substituted porphyrin: DFT and TDDFTâ€”PCM investigations. International Journal of Quantum Chemistry, 2011, 111, 2340-2351.	1.0	26
70	Hydrogen storage in TiO2 functionalized (10, 10) single walled carbon nanotube (SWCNT) â€“ First principles study. International Journal of Hydrogen Energy, 2014, 39, 4973-4980.	3.8	26
71	Three-dimensional oscillatory thermocapillary convection in liquid bridge under microgravity. International Journal of Heat and Mass Transfer, 2001, 44, 3765-3774.	2.5	25
72	Thiophene thiol on the Au(111) surface: Size-dependent adsorption study. Journal of Chemical Physics, 2003, 118, 9809-9813.	1.2	25

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73	Ab initiostudy of molecule transport characteristics based on nonequilibrium Greenâ€™s function theory. Physical Review B, 2005, 72, .	1.1	25
74	First Excited State Properties and Static Hyperpolarizability of Ruthenium(II) Ammine Complexes. Journal of Chemical Theory and Computation, 2006, 2, 1325-1334.	2.3	25
75	First-principles calculations of the far-infrared absorption spectrum of 4â€²-dimethylamino-N-methyl-4-stilbazolium tosylate. Chemical Physics Letters, 2006, 432, 157-162.	1.2	25
76	Chromate adsorption mechanism on nanodiamond-derived onion-like carbon. Journal of Hazardous Materials, 2016, 320, 368-375.	6.5	25
77	On the kinetics of the capillary imbibition of a simple fluid through a designed nanochannel using the molecular dynamics simulation approach. Journal of Colloid and Interface Science, 2010, 352, 566-572.	5.0	24
78	A theoretical study of the effects of transition metal dopants on the adsorption and dissociation of hydrogen on nickel clusters. International Journal of Quantum Chemistry, 2013, 113, 1940-1948.	1.0	24
79	Effect of nitrogen doping on titanium carbonitride-derived adsorbents used for arsenic removal. Journal of Hazardous Materials, 2016, 302, 375-385.	6.5	24
80	First Principles Calculation of Terahertz Vibrational Modes of a Disaccharide Monohydrate Crystal of Lactose. Japanese Journal of Applied Physics, 2006, 45, L1156-L1158.	0.8	23
81	Gate-induced switching and negative differential resistance in a single-molecule transistor: Emergence of fixed and shifting states with molecular length. Journal of Chemical Physics, 2007, 127, 024901.	1.2	23
82	Theoretical study of hydrogen storage in binary hydrogen-methane clathrate hydrates. Journal of Renewable and Sustainable Energy, 2014, 6, .	0.8	23
83	Computational study on the interactions of mustard gas with cucurbituril macrocycles. International Journal of Quantum Chemistry, 2015, 115, 1515-1525.	1.0	23
84	Terahertz Vibrational Modes of Crystalline Salicylic Acid by Numerical Model Using Periodic Density Functional Theory. Japanese Journal of Applied Physics, 2006, 45, 4170-4175.	0.8	22
85	Control of Electron Transport by Manipulating the Conjugated Framework. Journal of Physical Chemistry C, 2007, 111, 15397-15403.	1.5	22
86	Impact of type of crystal defects in multicrystalline Si on electrical properties and interaction with impurities. Journal of Applied Physics, 2011, 109, .	1.1	22
87	Computational discovery of a new rhombohedral diamond phase. Physical Review B, 2018, 98, .	1.1	22
88	Effect of substituent groups on the electronic properties of a molecular device: an ab initio theoretical study. Computational and Theoretical Chemistry, 2004, 681, 65-69.	1.5	21
89	Dynamical Criteria for Cs Ion Insertion and Adsorption at Cap and Stem of Carbon Nanotubes:Â Ab Initio Study and Comparison with Experiment. Journal of Physical Chemistry B, 2004, 108, 15529-15535.	1.2	21
90	Band-Structure Design of Fluoride Complex Materials for Deep-Ultraviolet Light-Emitting Diodes. Japanese Journal of Applied Physics, 2005, 44, 7285-7290.	0.8	21

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91	Dynamic Ad-Dimer Twisting Assisted Nanowire Self-Assembly on Si(001). Physical Review Letters, 2005, 94, 226103.	2.9	21
92	Electronic and transport properties of bismuth nanolines for applications in molecular electronics. Physical Review B, 2007, 75, .	1.1	21
93	Modification of graphene as active hydrogen storage medium by strain engineering. Computational Materials Science, 2012, 65, 144-148.	1.4	21
94	Body centered cubic carbon BC14: An all- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>s</mml:mi><mml:msup><mml:mi>p</mml:mi><mml:mn> bonded full-fledged pentadiamond. Physical Review B, 2020, 102, .	1.1	21
95	Molecular Resistance in a Molecular Diode:Â A Case Study of the Substituted Phenylethynyl Oligomer. Journal of Physical Chemistry A, 2002, 106, 7911-7914.	1.1	20
96	Design Proposal of Light Emitting Diode in Vacuum Ultraviolet Based on Perovskite-Like Fluoride Crystals. Japanese Journal of Applied Physics, 2004, 43, L1140-L1143.	0.8	20
97	Theoretical modelling of the phase diagrams of clathrate hydrates for hydrogen storage applications. Molecular Simulation, 2012, 38, 773-780.	0.9	20
98	Birefringence of Î²-BaB2O4 crystal in the terahertz region for parametric device design. Applied Physics Letters, 2008, 92, .	1.5	19
99	Highly stable and symmetric boron caged B@Co12@B80 core-shell cluster. Applied Physics Letters, 2009, 94, 133102.	1.5	19
100	Effects of Alkali Adatoms on CO and H₂S Adsorptions on the Fe(100) Surface: A Density Functional Theory Study. Journal of Physical Chemistry C, 2011, 115, 23893-23901.	1.5	19
101	An ideal polymeric C60 coating on a Si electrode for durable Li-ion batteries. Carbon, 2014, 77, 1140-1147.	5.4	19
102	A superhard orthorhombic carbon with all six-membered-ring in sp3 bonding networks. Physics Letters, Section A: General, Atomic and Solid State Physics, 2019, 383, 2809-2812.	0.9	19
103	Molecular Enamel Wires for Electronic Devices: Theoretical Study. Japanese Journal of Applied Physics, 2003, 42, 2492-2494.	0.8	18
104	Cluster growth processes by direct simulation monte carlo method. Applied Physics A: Materials Science and Processing, 2001, 73, 731-735.	1.1	17
105	Ionization potentials of small tin clusters: first principles calculations. Chemical Physics Letters, 2002, 356, 36-42.	1.2	17
106	Stability of Sb line structures on Si(001). Physical Review B, 2003, 67, .	1.1	17
107	Realization of molecular interconnection for molecular electronics: Theoretical aspects. Computational Materials Science, 2006, 36, 130-134.	1.4	17
108	HYDROGEN STORAGE ON NANOFULLERENE CAGES. Nano, 2009, 04, 253-263.	0.5	17

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109	Effects of hydration level, temperature, side chain and backbone flexibility of the polymer on the proton transfer in short-side-chain perfluorosulfonic acid membranes at low humidity conditions. Journal of Membrane Science, 2011, 369, 339-349.	4.1	16
110	Effects of rotating magnetic fields on thermocapillary flow in a floating half-zone. Journal of Crystal Growth, 2011, 316, 177-184.	0.7	16
111	First-principles analysis of structural and opto-electronic properties of indium tin oxide. Journal of Applied Physics, 2012, 111, .	1.1	16
112	Theoretical study of the alkyl derivative C 37 H 50 N 4 O 4 molecule for use as a stable molecular rectifier: geometric and electronic structures. Computational Materials Science, 2003, 27, 161-165.	1.4	15
113	Electronic transport properties of a metalâ€“semiconductor carbon nanotube heterojunction. Physica E: Low-Dimensional Systems and Nanostructures, 2004, 22, 675-678.	1.3	15
114	Self-consistent study of single molecular transistor modulated by transverse field. Journal of Chemical Physics, 2006, 125, 084710.	1.2	15
115	Growth processes of magnetic clusters studied by direct simulation Monte Carlo method. Journal of Applied Physics, 2000, 87, 6561-6563.	1.1	14
116	Theoretical study of insulated wires based on polymer chains encapsulated in molecular nanotubes. Thin Solid Films, 2003, 438-439, 80-84.	0.8	14
117	Ab InitioStudy of Divalent 3dTransition Metal Impurities in KMgF3and BaLiF3. Japanese Journal of Applied Physics, 2003, 42, 5082-5085.	0.8	14
118	Theoretical Study of Chlorin-Fullerene Supramolecular Complexes for Photovoltaic Devices. Japanese Journal of Applied Physics, 2003, 42, 2503-2505.	0.8	14
119	Theoretical investigation of hydrogen storage ability of a carbon nanohorn. Computational Materials Science, 2010, 49, S378-S382.	1.4	14
120	First-principles study of the H2 splitting processes on pure and transition-metal-doped Al (111) surfaces. International Journal of Hydrogen Energy, 2011, 36, 12742-12752.	3.8	14
121	Body-centered-cubic lattice model with many-body interactions representing the melting transition in Si. Journal of Chemical Physics, 1999, 110, 9608-9617.	1.2	13
122	Site-Percolation Models Including Heterogeneous Particles on a Square Lattice. Materials Transactions, JIM, 1999, 40, 1314-1318.	0.9	13
123	Usefulness of experiments with model fluid for thermocapillary convectionâ€"effect of Prandtl number on two-dimensional thermocapillary convection. Journal of Crystal Growth, 2002, 234, 272-278.	0.7	13
124	Electron Transport in Molecular Enamel Wires. Japanese Journal of Applied Physics, 2004, 43, 2061-2063.	0.8	13
125	Ab initioDetermination of Total-Energy Surfaces for Distortions of Ferroelectric Perovskite Oxides. Japanese Journal of Applied Physics, 2004, 43, 6785-6792.	0.8	13
126	Electronic and Transport Properties of Ferrocene: Theoretical Study. Japanese Journal of Applied Physics, 2006, 45, 3768-3771.	0.8	13

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127	Ab initiostudy of single-molecule rotation switch based on nonequilibrium Greenâ€™s function theory. Journal of Chemical Physics, 2007, 127, 084107.	1.2	13
128	Interstitial Oxygen and Dopant Atoms Arrangement in Tin-Doped Indium Oxide. Materials Transactions, 2007, 48, 666-669.	0.4	13
129	Numerical simulation of crucible rotation in high-temperature solution growth method using a Fourier-Legendre spectral element method. International Journal of Heat and Mass Transfer, 2013, 64, 882-891.	2.5	13
130	Sources ofn-type conductivity in GaInO₃. Journal Physics D: Applied Physics, 2015, 48, 015101.	1.3	13
131	Weak Universality of a Site-Percolation Model with Two Different Sizes of Particles on a Square Lattice. Journal of the Physical Society of Japan, 1999, 68, 3755-3758.	0.7	12
132	Thermodynamic properties of the Cuâ€“Au system using a face-centered-cubic lattice model with a renormalized potential. Journal of Chemical Physics, 2004, 120, 9297-9301.	1.2	12
133	Prediction and analysis of flow behavior of a polymer melt through nanochannels using artificial neural network and statistical methods. Microfluidics and Nanofluidics, 2010, 9, 319-328.	1.0	12
134	Effects of rotating magnetic fields on thermocapillary flow: Comparison of the infinite and the Î¦1â€“Î¦2 models. International Journal of Thermal Sciences, 2010, 49, 2413-2418.	2.6	12
135	First principles calculation of La3Ta0.5Ga5.5O14 crystal with acceptor-like intrinsic point defects. Journal of Applied Physics, 2010, 108, 113505.	1.1	12
136	Rigid adamantane tripod linkage for well-defined conductance of a single-molecule junction. Physical Chemistry Chemical Physics, 2010, 12, 11763.	1.3	12
137	Single walled carbon nanotubes functionalized with hydrides as potential hydrogen storage media: A survey of intermolecular interactions. Physica Status Solidi (B): Basic Research, 2011, 248, 2147-2158.	0.7	12
138	Theoretical study of donorâ€“spacerâ€“acceptor structure molecule for use as stable molecular rectifier: geometric and electronic structures. Thin Solid Films, 2003, 438-439, 235-237.	0.8	11
139	ab initioStudy of Strain-Induced Ferroelectricity in SrTiO3. Japanese Journal of Applied Physics, 2005, 44, 7134-7140.	0.8	11
140	Controlling the Percolation Threshold of Conductor-Insulator Composites by Changing the Granular Size of Insulators. Materials Transactions, 2010, 51, 1141-1144.	0.4	11
141	First principles study on desorption of chemisorbed hydrogen atoms from single-walled carbon nanotubes under external electric field. International Journal of Hydrogen Energy, 2011, 36, 13645-13656.	3.8	11
142	Thermal Behavior of Caged Silsesquioxane (POSS) Studied by Molecular Dynamics Simulations. Journal of Inorganic and Organometallic Polymers and Materials, 2012, 22, 845-851.	1.9	11
143	A comparative study of lattice Boltzmann models for incompressible flow. Computers and Mathematics With Applications, 2014, 68, 1446-1466.	1.4	11
144	Onion-like carbon as dopant/modification-free electrocatalyst for [VO]2+/[VO2]+ redox reaction: Performance-control mechanism. Carbon, 2018, 127, 31-40.	5.4	11

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145	Electron transport through heterocyclic molecule: ab initio molecular orbital theory. Physics Letters, Section A: General, Atomic and Solid State Physics, 2004, 326, 412-416.	0.9	10
146	Electronic and Transport Properties of Doped Organic Molecules for Molecular Wire Applications. Japanese Journal of Applied Physics, 2005, 44, 2823-2825.	0.8	10
147	Two-Stage Rotation Mechanism for Group-V Precursor Dissociation on Si(001). Physical Review Letters, 2006, 97, 046103.	2.9	10
148	Electronic and magnetic properties of double-impurities-doped TiO2 (rutile): First-principles calculations. Journal of Applied Physics, 2006, 99, 08M105.	1.1	10
149	A novel computational approach to study proton transfer in perfluorosulfonic acid membranes. International Journal of Hydrogen Energy, 2010, 35, 3648-3655.	3.8	10
150	First-Principles Calculations on Î£3 Grain Boundary Transition Metal Impurities in Multicrystalline Silicon. Japanese Journal of Applied Physics, 2010, 49, 04DP02.	0.8	10
151	Electron transport characteristics of organic molecule encapsulated carbon nanotubes. Nanoscale, 2011, 3, 1773.	2.8	10
152	Gate-controlled current and inelastic electron tunneling spectrum of benzene: A self-consistent study. Journal of Chemical Physics, 2011, 134, 144113.	1.2	10
153	Transport Properties of Nanoscale Materials for Molecular Wire Applications: A Case Study of Ferrocene Dimers. Journal of the Korean Physical Society, 2008, 52, 1197-1201.	0.3	10
154	Simulation of electrochemical deposition process by a multiparticle diffusive aggregation model. Journal of Applied Physics, 2000, 87, 4611-4616.	1.1	9
155	Theoretical Analysis for a Molecular Resonant Tunneling Diode. Japanese Journal of Applied Physics, 2002, 41, 2770-2773.	0.8	9
156	Excess polarizabilities upon excitation from the ground state to the first dipole-allowed excited state of diphenylpolyenes. International Journal of Quantum Chemistry, 2007, 107, 2006-2014.	1.0	9
157	Crystal-like low frequency phonons in the low-density amorphous and high-density amorphous ices. Journal of Chemical Physics, 2008, 129, 114507.	1.2	9
158	An efficient tool for modeling and predicting fluid flow in nanochannels. Journal of Chemical Physics, 2009, 131, 184506.	1.2	9
159	First principles investigation on carbon nanostructures functionalized with borane: An analysis on their hydrogen storage capacity. Physica E: Low-Dimensional Systems and Nanostructures, 2011, 43, 1528-1534.	1.3	9
160	A new model of DLA under high magnetic field. Computational Materials Science, 1998, 10, 46-50.	1.4	8
161	NUMERICAL STUDY OF DYNAMIC BEHAVIOR OF MELTING SAMPLE IN SHEAR CELL UNDER MICROGRAVITY. Numerical Heat Transfer; Part A: Applications, 1998, 34, 709-718.	1.2	8
162	A new crystal growth model based on a stochastic method under an external field. Modelling and Simulation in Materials Science and Engineering, 2000, 8, 1-11.	0.8	8

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163	Multiscale simulation of cluster growth and deposition processes by hybrid model based on direct simulation Monte Carlo method. Computational Materials Science, 2002, 24, 88-92.	1.4	8
164	Molecular orbital analysis of frontier orbitals for molecular electronics: a case study of unimolecular rectifier and photovoltaic cell. Science and Technology of Advanced Materials, 2003, 4, 377-382.	2.8	8
165	THEORETICAL STUDY OF MOLECULAR ENAMEL WIRES BASED ON POLYTHIOPHENE-CYCLODEXTRIN INCLUSION COMPLEXES. Molecular Crystals and Liquid Crystals, 2003, 406, 1-10.	0.4	8
166	Three-dimensional unsteady convection in LiCaAlF6-Czochralski growth. Journal of Crystal Growth, 2004, 266, 81-87.	0.7	8
167	Electron transport through molecular wire: effect of isomery. Physica E: Low-Dimensional Systems and Nanostructures, 2005, 25, 643-646.	1.3	8
168	Transition between N- and Z-shaped current-voltage characteristics in semiconductor multiple-quantum-well structures. Journal of Applied Physics, 2006, 100, 033718.	1.1	8
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