Seungwu Han

List of Publications by Year in Descending Order

149 papers	7,099 citations	41 h-index	81 g-index
155 ext. papers	7,962 ext. citations	7.1 avg, IF	5.77 L-index

#	Paper	IF	Citations
149	Understanding the Role of Electronic Effects in CO on the Pt3Sn Alloy Surface via Band Structure Measurements. *ACS Catalysis*, **2022**, 12, 219-225	13.1	3
148	Accelerated computation of lattice thermal conductivity using neural network interatomic potentials. *Computational Materials Science*, **2022**, 211, 111472	3.2	0
147	Field-like spin–orbit torque induced by bulk Rashba channels in GeTe/NiFe bilayers. *NPG Asia Materials*, **2021**, 13,	10.3	2
146	High-dimensional neural network atomic potentials for examining energy materials: some recent simulations. *JPhys Energy*, **2021**, 3, 012003	4.9	5
145	Identification of Active Sites for CO Reduction on Graphene-Supported Single-Atom Catalysts. *ChemSusChem*, **2021**, 14, 2475-2480	8.3	2
144	Density Functional Theory Study of Edge-Induced Atomic-Scale Structural Phase Transitions of MoS2 Nanocrystals: Implications for a High-Performance Catalyst. *ACS Applied Nano Materials*, **2021**, 4, 5496-5502	5.6	2
143	Best practices in machine learning for chemistry. *Nature Chemistry*, **2021**, 13, 505-508	17.6	61
142	Triboelectrification: Backflow and Stuck Charges Are Key. *ACS Energy Letters*, **2021**, 6, 2792-2799	20.1	7
141	Tailoring topological Hall effect in SrRuO3/SrTiO3 superlattices. *Acta Materialia*, **2021**, 216, 117153	8.4	3
140	One-dimensional structures of three quinone molecules on Au(111). *Surface Science*, **2021**, 713, 121911	1.8	0
139	Production of C, N Alternating 2D Materials Using Covalent Modification and Their Electroluminescence Performance. *Small Science*, **2021**, 1, 2000042		4
138	Origin of p-Type Conduction in Amorphous CuI: A First-Principles Investigation. *Physica Status Solidi (B): Basic Research*, **2020**, 257, 2000218	1.3	3
137	AMP2: A fully automated program for ab initio calculations of crystalline materials. *Computer Physics Communications*, **2020**, 256, 107450	4.2	4
136	Effects of the Heterointerface on the Growth Characteristics of a Brownmillerite SrFeO Thin Film Grown on SrRuO and SrTiO Perovskites. *Scientific Reports*, **2020**, 10, 3807	4.9	7
135	Crystallization of amorphous GeTe simulated by neural network potential addressing medium-range order. *Computational Materials Science*, **2020**, 181, 109725	3.2	11
134	Fundamental Limit of the Emission Linewidths of Quantum Dots: An Ab Initio Study of CdSe Nanocrystals. *ACS Applied Materials & Interfaces*, **2020**, 12, 22012-22018	9.5	5
133	Training machine-learning potentials for crystal structure prediction using disordered structures. *Physical Review B*, **2020**, 102,	3.3	2

132	Efficient Atomic-Resolution Uncertainty Estimation for Neural Network Potentials Using a Replica Ensemble. *Journal of Physical Chemistry Letters*, **2020**, 11, 6090-6096	6.4	8
131	A band-gap database for semiconducting inorganic materials calculated with hybrid functional. *Scientific Data*, **2020**, 7, 387	8.2	8
130	Computational Identification of Transition-Metal Dichalcogenides for Electrochemical CO2 Reduction to Highly Reduced Species Beyond CO and HCOOH. *Journal of Physical Chemistry C*, **2020**, 124, 25812-25820	3.8	6
129	Adatom Doping of Transition Metals in ReSe Nanosheets for Enhanced Electrocatalytic Hydrogen Evolution Reaction. *ACS Nano*, **2020**, 14, 12184-12194	16.7	21
128	Antiperovskite Oxides as Promising Candidates for High-Performance Ferroelectric Photovoltaics: First-Principles Investigation on BaAsO and BaSbO. *ACS Applied Materials & Interfaces*, **2020**, 12, 43798-43804	9.5	4
127	Indium-Free Amorphous Ca□Al□O Thin Film as a Transparent Conducting Oxide. *Chemistry of Materials*, **2019**, 31, 8019-8025	9.6	6
126	Boosting the photocatalytic hydrogen evolution performance via an atomically thin 2D heterojunction visualized by scanning photoelectrochemical microscopy. *Nano Energy*, **2019**, 65, 104053	17.1	11
125	Material Design of New p-Type Tin Oxyselenide Semiconductor through Valence Band Engineering and Its Device Application. *ACS Applied Materials & Interfaces*, **2019**, 11, 40214-40221	9.5	9
124	First-principles calculations on effects of Al and Ga dopants on atomic and electronic structures of amorphous Ge2Sb2Te5. *Journal of Applied Physics*, **2019**, 125, 035701	2.5	2
123	A molecular dynamics study on the interface morphology of vapor-deposited amorphous organic thin films. *Physical Chemistry Chemical Physics*, **2019**, 21, 1484-1490	3.6	7
122	Computational Screening of Indirect-Gap Semiconductors for Potential Photovoltaic Absorbers. *Chemistry of Materials*, **2019**, 31, 4072-4080	9.6	10
121	SIMPLE-NN: An efficient package for training and executing neural-network interatomic potentials. *Computer Physics Communications*, **2019**, 242, 95-103	4.2	40
120	Unveiling Electrochemical Reaction Pathways of CO Reduction to C Species at S-Vacancies of MoS. *ChemSusChem*, **2019**, 12, 2671-2678	8.3	16
119	Large-Scale Computational Identification of p-Type Oxide Semiconductors by Hierarchical Screening. *Chemistry of Materials*, **2019**, 31, 5475-5483	9.6	11
118	Two-Dimensional NbS Gas Sensors for Selective and Reversible NO Detection at Room Temperature. *ACS Sensors*, **2019**, 4, 2395-2402	9.2	57
117	Anion Extraction-Induced Polymorph Control of Transition Metal Dichalcogenides. *Nano Letters*, **2019**, 19, 8644-8652	11.5	9
116	Atomic energy mapping of neural network potential. *Physical Review Materials*, **2019**, 3,	3.2	14
115	Lanthanum Doping Enabling High Drain Current Modulation in a p-Type Tin Monoxide Thin-Film Transistor. *ACS Applied Materials & Interfaces*, **2019**, 11, 47025-47036	9.5	16

114	The Nature of the Oxygen Vacancy in Amorphous Oxide Semiconductors: Shallow Versus Deep. *Physica Status Solidi (B): Basic Research*, **2019**, 256, 1800486	1.3	10
113	Computational discovery of p-type transparent oxide semiconductors using hydrogen descriptor. *Npj Computational Materials*, **2018**, 4,	10.9	45
112	One-pot synthesis of sulfur and nitrogen codoped titanium dioxide nanorod arrays for superior photoelectrochemical water oxidation. *Applied Catalysis B: Environmental*, **2018**, 234, 213-222	21.8	24
111	Hydrogen Evolution Reaction at Anion Vacancy of Two-Dimensional Transition-Metal Dichalcogenides: Ab Initio Computational Screening. *Journal of Physical Chemistry Letters*, **2018**, 9, 2049-2055	6.4	62
110	Role of Hyper-Reduced States in Hydrogen Evolution Reaction at Sulfur Vacancy in MoS2. *ACS Catalysis*, **2018**, 8, 4508-4515	13.1	28
109	Effect of annealing temperature on the phase transition, band gap and thermoelectric properties of Cu2SnSe3. *Journal of Materials Chemistry C*, **2018**, 6, 1780-1788	7.1	21
108	Directly Assembled 3D Molybdenum Disulfide on Silicon Wafer for Efficient Photoelectrochemical Water Reduction. *Advanced Sustainable Systems*, **2018**, 2, 1700142	5.9	30
107	All-atom simulation of molecular orientation in vapor-deposited organic light-emitting diodes. *Journal of Materials Chemistry C*, **2018**, 6, 1015-1022	7.1	25
106	Two-dimensional networks of brominated Y-shaped molecules on Au(111). *Applied Surface Science*, **2018**, 432, 332-336	6.7	7
105	Networks of non-planar molecules with halogen bonds studied using scanning tunneling microscopy on Au (111). *Applied Surface Science*, **2018**, 432, 110-114	6.7	5
104	Effect of Nb concentration on the spin-orbit coupling strength in Nb-doped SrTiO epitaxial thin films. *Scientific Reports*, **2018**, 8, 5739	4.9	1
103	Toward Reliable and Transferable Machine Learning Potentials: Uniform Training by Overcoming Sampling Bias. *Journal of Physical Chemistry C*, **2018**, 122, 22790-22795	3.8	16
102	High-throughput ab initio calculations on dielectric constant and band gap of non-oxide dielectrics. *Scientific Reports*, **2018**, 8, 14794	4.9	10
101	First-principles study on the negative-U behavior of K centers in amorphous Si3N4. *Physical Review Applied*, **2018**, 10,	4.3	4
100	Intrinsic Carrier Mobility of Cesium Lead Halide Perovskites. *Physical Review Applied*, **2018**, 10,	4.3	41
99	Double-Layer Graphene Outperforming Monolayer as Catalyst on Silicon Photocathode for Hydrogen Production. *ACS Applied Materials & Interfaces*, **2017**, 9, 3570-3580	9.5	15
98	Property database for single-element doping in ZnO obtained by automated first-principles calculations. *Scientific Reports*, **2017**, 7, 40907	4.9	55
97	An origin of unintentional doping in transition metal dichalcogenides: the role of hydrogen impurities. *Nanoscale*, **2017**, 9, 4265-4271	7.7	18

96	Cu Diffusion-Driven Dynamic Modulation of the Electrical Properties of Amorphous Oxide Semiconductors. *Advanced Functional Materials*, **2017**, 27, 1700336	15.6	6
95	Drastically enhanced hydrogen evolution activity by 2D to 3D structural transition in anion-engineered molybdenum disulfide thin films for efficient Si-based water splitting photocathodes. *Journal of Materials Chemistry A*, **2017**, 5, 15534-15542	13	57
94	Identification of ground-state spin ordering in antiferromagnetic transition metal oxides using the Ising model and a genetic algorithm. *Science and Technology of Advanced Materials*, **2017**, 18, 246-252	7.1	15
93	Oxygen Vacancy Linear Clustering in a Perovskite Oxide. *Journal of Physical Chemistry Letters*, **2017**, 8, 3500-3505	6.4	30
92	Origin of Electrical Instabilities in Self-Aligned Amorphous InGaZnO Thin-Film Transistors. *IEEE Transactions on Electron Devices*, **2017**, 64, 4965-4973	2.9	24
91	Ab initio calculation of ionization potential and electron affinity in solid-state organic semiconductors. *Physical Review B*, **2016**, 93,	3.3	20
90	Atomic Structure and Spectroscopy of Single Metal (Cr, V) Substitutional Dopants in Monolayer MoS. *ACS Nano*, **2016**, 10, 10227-10236	16.7	77
89	Light-Induced Peroxide Formation in ZnO: Origin of Persistent Photoconductivity. *Scientific Reports*, **2016**, 6, 35148	4.9	20
88	Emergence of Negative Capacitance in Multidomain Ferroelectric-Paraelectric Nanocapacitors at Finite Bias. *Advanced Materials*, **2016**, 28, 335-40	24	28
87	Organolead Halide Perovskites for Low Operating Voltage Multilevel Resistive Switching. *Advanced Materials*, **2016**, 28, 6562-7	24	219
86	Ultrasensitive reversible oxygen sensing by using liquid-exfoliated MoS2 nanoparticles. *Journal of Materials Chemistry A*, **2016**, 4, 6070-6076	13	61
85	Wafer-scale transferable molybdenum disulfide thin-film catalysts for photoelectrochemical hydrogen production. *Energy and Environmental Science*, **2016**, 9, 2240-2248	35.4	150
84	Structure of amorphous GeSe9 by neutron diffraction and first-principles molecular dynamics: Impact of trajectory sampling and size effects. *Journal of Chemical Physics*, **2016**, 145, 084502	3.9	6
83	Novel high- dielectrics for next-generation electronic devices screened by automated ab initio calculations. *NPG Asia Materials*, **2015**, 7, e190-e190	10.3	106
82	Origin of degradation phenomenon under drain bias stress for oxide thin film transistors using IGZO and IGO channel layers. *Scientific Reports*, **2015**, 5, 7884	4.9	26
81	Hydrogen Bistability as the Origin of Photo-Bias-Thermal Instabilities in Amorphous Oxide Semiconductors. *Advanced Electronic Materials*, **2015**, 1, 1400006	6.4	64
80	Investigation of field effects in a solid-state nanopore transistor. *Physical Chemistry Chemical Physics*, **2015**, 17, 27806-11	3.6	5
79	First-principles calculation of charged capacitors under open-circuit conditions using the orbital-separation approach. *Physical Review B*, **2015**, 92,	3.3	2

78	Source of instability at the amorphous interface between InGaZnO and SiO: A theoretical investigation. *Physica Status Solidi (B): Basic Research*, **2015**, 252, 1872-1876	1.3	10
77	Nature of chemical states of sulfur embedded in atomic-layer-deposited HfO2 film on Ge substrate for interface passivation. *Physica Status Solidi - Rapid Research Letters*, **2015**, 9, 511-515	2.5	2
76	Origin of the improved mobility and photo-bias stability in a double-channel metal oxide transistor. *Scientific Reports*, **2014**, 4, 3765	4.9	81
75	GW calculations on post-transition-metal oxides. *Physical Review B*, **2014**, 89,	3.3	15
74	Effect of oxygen vacancy on the structural and electronic characteristics of crystalline Zn2SnO4. *Journal of Materials Chemistry C*, **2014**, 2, 8381-8387	7.1	13
73	The impact of orbital hybridization on the electronic structure of crystalline InGaZnO: a new perspective on the compositional dependence. *Journal of Materials Chemistry C*, **2014**, 2, 9196-9204	7.1	18
72	Hydrated manganese(II) phosphate (Mn(PO)3HO) as a water oxidation catalyst. *Journal of the American Chemical Society*, **2014**, 136, 7435-43	16.4	266
71	An efficient method to generate amorphous structures based on local geometry. *Computational Materials Science*, **2014**, 95, 256-262	3.2	14
70	Intrinsic nature of visible-light absorption in amorphous semiconducting oxides. *APL Materials*, **2014**, 2, 032108	5.7	19
69	Supramolecular Cl???H and O???H interactions in self-assembled 1,5-dichloroanthraquinone layers on Au(111). *ChemPhysChem*, **2013**, 14, 1177-81	3.2	18
68	Cation disorder as the major electron scattering source in crystalline InGaZnO. *Applied Physics Letters*, **2013**, 102, 152104	3.4	22
67	N-doped monolayer graphene catalyst on silicon photocathode for hydrogen production. *Energy and Environmental Science*, **2013**, 6, 3658	35.4	119
66	Role of preferential weak hybridization between the surface-state of a metal and the oxygen atom in the chemical adsorption mechanism. *Physical Chemistry Chemical Physics*, **2013**, 15, 19019-23	3.6	6
65	Thermodynamics of native point defects in Fe2O3: an ab initio study. *Physical Chemistry Chemical Physics*, **2013**, 15, 18906-14	3.6	76
64	Supramolecular interactions of anthraquinone networks on Au(111): Hydrogen bonds and van der Waals interactions. *Applied Surface Science*, **2013**, 268, 432-435	6.7	9
63	Role of Transition Metal in Fast Oxidation Reaction on the Pt3TM (111) (TM = Ni, Co) Surfaces. *Advanced Energy Materials*, **2013**, 3, 1257-1261	21.8	32
62	Molecular Multistate Systems Formed in Two-Dimensional Porous Networks on Ag(111). *Journal of Physical Chemistry C*, **2013**, 117, 302-306	3.8	27
61	Ab initio study on the structural characteristics of amorphous Zn2SnO4. *Applied Physics Letters*, **2013**, 103, 252102	3.4	8

60	Competing local orders in liquid and amorphous structures of Ge2Sb2Te5: Influence of exchange-correlation functional. *Journal of Applied Physics*, **2013**, 113, 134302	2.5	10
59	Stabilization of Tetragonal HfO2 under Low Active Oxygen Source Environment in Atomic Layer Deposition. *Chemistry of Materials*, **2012**, 24, 3534-3543	9.6	64
58	Fast and scalable memory characteristics of Ge-doped SbTe phase change materials. *Physica Status Solidi (B): Basic Research*, **2012**, 249, 1985-1991	1.3	15
57	Microscopic origin of universal quasilinear band structures of transparent conducting oxides. *Physical Review Letters*, **2012**, 108, 196404	7.4	23
56	The Impact of Carbon Concentration on the Crystalline Phase and Dielectric Constant of Atomic Layer Deposited HfO2Films on Ge Substrate. *ECS Journal of Solid State Science and Technology*, **2012**, 1, N33-N37	2	20
55	A detailed understanding of the electronic bipolar resistance switching behavior in Pt/TiO2/Pt structure. *Nanotechnology*, **2011**, 22, 254010	3.4	140
54	Electronic structure of Pt/HfO2 interface with oxygen vacancy. *Microelectronic Engineering*, **2011**, 88, 3407-3410	2.5	5
53	Hybrid functional study on structural and electronic properties of oxides. *Current Applied Physics*, **2011**, 11, S337-S340	2.6	50
52	A microscopic model for resistance drift in amorphous Ge2Sb2Te5. *Current Applied Physics*, **2011**, 11, e82-e84	2.6	9
51	Multiscale simulation on electromigration of the oxygen vacancies in metal oxides. *Applied Physics A: Materials Science and Processing*, **2011**, 102, 909-914	2.6	6
50	A simple device unit consisting of all NiO storage and switch elements for multilevel terabit nonvolatile random access memory. *ACS Applied Materials & Interfaces*, **2011**, 3, 4475-9	9.5	26
49	Interchain Interactions Mediated by Br Adsorbates in Arrays of Metal□Organic Hybrid Chains on Ag(111). *Journal of Physical Chemistry C*, **2011**, 115, 14834-14838	3.8	62
48	Visualizing Halogen Bonds in Planar Supramolecular Systems. *Journal of Physical Chemistry C*, **2011**, 115, 2297-2301	3.8	61
47	Influence of exchange-correlation functionals on dielectric properties of rutile TiO2. *Current Applied Physics*, **2011**, 11, S293-S296	2.6	22
46	Enhanced amorphous stability of carbon-doped Ge2Sb2Te5: Ab Initio investigation. *Applied Physics Letters*, **2011**, 99, 183501	3.4	47
45	Ab initio study on influence of dopants on crystalline and amorphous Ge2Sb2Te5. *Journal of Applied Physics*, **2011**, 109, 043705-043705-10	2.5	43
44	Achieving chiral resolution in self-assembled supramolecular structures through kinetic pathways. *Nanotechnology*, **2011**, 22, 275705	3.4	21
43	Atomic structure of conducting nanofilaments in TiO2 resistive switching memory. *Nature Nanotechnology*, **2010**, 5, 148-53	28.7	1672

42	Effects of pressure on atomic and electronic structure and crystallization dynamics of amorphous Ge2Sb2Te5. *Physical Review B*, **2010**, 81,	3.3	29
41	First-principles study of preferential sites of hydrogen incorporated in epitaxial graphene on 6H-SiC(0001). *Physical Review B*, **2010**, 81,	3.3	40
40	Hydrogen adsorption and carrier generation in LaAlO3-SrTiO3 heterointerfaces: a first-principles study. *Journal of Physics Condensed Matter*, **2010**, 22, 315501	1.8	30
39	Reduction of Electrical Defects in Atomic Layer Deposited HfO2 Films by Al Doping. *Chemistry of Materials*, **2010**, 22, 4175-4184	9.6	52
38	Field Emission Theory **2010**, 41-54		
37	Novel bi-nuclear boron complex with pyrene ligand: red-light emitting as well as electron transporting material in organic light-emitting diodes. *Organic Letters*, **2010**, 12, 1272-5	6.2	80
36	Capacitors with an Equivalent Oxide Thickness of . *Advanced Functional Materials*, **2010**, 20, 2989-3003	15.6	160
35	Mapping the electronic structures of a metalloporphyrin molecule on Au(111) by scanning tunneling microscopy and spectroscopy. *Physical Review B*, **2009**, 80,	3.3	19
34	Change in the resistivity of Ge-doped Sb phase change thin films grown by chemical vapor deposition according to their microstructures. *Applied Physics Letters*, **2009**, 94, 222115	3.4	4
33	Microscopic origin of current degradation of fully-sealed carbon-nanotube field emission display. *Solid State Communications*, **2009**, 149, 670-672	1.6	9
32	Improved field emission properties of double-walled carbon nanotubes decorated with Ru nanoparticles. *Carbon*, **2009**, 47, 1158-1164	10.4	103
31	Electrical manipulation of nanofilaments in transition-metal oxides for resistance-based memory. *Nano Letters*, **2009**, 9, 1476-81	11.5	354
30	Phase stability and electronic structures of stoichiometric tantalum mononitrides. *Computational Materials Science*, **2008**, 44, 577-580	3.2	14
29	Segregation of oxygen vacancy at metal-HfO2 interfaces. *Applied Physics Letters*, **2008**, 92, 233118	3.4	30
28	Electronic structure tailoring and selective adsorption mechanism of metal-coated nanotubes. *Nano Letters*, **2008**, 8, 81-6	11.5	40
27	Al-Doped TiO2 Films with Ultralow Leakage Currents for Next Generation DRAM Capacitors. *Advanced Materials*, **2008**, 20, 1429-1435	24	248
26	Dielectric Properties of Ultrathin SrTiO3 and Metal-SrTiO3 Interfaces. *Journal of the Korean Physical Society*, **2008**, 52, 70-74	0.6	4
25	Pairing of cation vacancies and gap-state creation in TiO2 and HfO2. *Applied Physics Letters*, **2007**, 90, 252908	3.4	21

24	Field emission of metal nanowires studied by first-principles methods. *Nanotechnology*, **2007**, 18, 475706	3.4	15
23	Oxygen vacancy clustering and electron localization in oxygen-deficient SrTiO(3): LDA + U study. *Physical Review Letters*, **2007**, 98, 115503	7.4	244
22	Effects of carbon residue in atomic layer deposited HfO2 films on their time-dependent dielectric breakdown reliability. *Applied Physics Letters*, **2007**, 90, 182907	3.4	46
21	Influence of carrier injection on resistive switching of TiO2 thin films with Pt electrodes. *Applied Physics Letters*, **2006**, 89, 162912	3.4	62
20	Band-gap sensitive adsorption of fluorine molecules on sidewalls of carbon nanotubes: an ab initio study. *Nanotechnology*, **2006**, 17, 5862-5865	3.4	5
19	Ab initiostudy of the effect of nitrogen on carbon nanotube growth. *Nanotechnology*, **2006**, 17, 909-912	3.4	13
18	Ab initio study on the carbon nanotube with various degrees of functionalization. *Chemical Physics Letters*, **2006**, 419, 134-138	2.5	23
17	Chirality- and diameter-dependent reactivity of NO2 on carbon nanotube walls. *Journal of the American Chemical Society*, **2005**, 127, 15724-9	16.4	84
16	Selective removal of metallic single-walled carbon nanotubes with small diameters by using nitric and sulfuric acids. *Journal of Physical Chemistry B*, **2005**, 109, 19242-8	3.4	98
15	Band gap sensitivity of bromine adsorption at carbon nanotubes. *Chemical Physics Letters*, **2005**, 403, 135-139	2.5	29
14	Ferromagnetism at the edges of the stacked graphitic fragments: an ab initio study. *Chemical Physics Letters*, **2004**, 398, 207-211	2.5	36
13	Field emission properties of carbon nanotubes coated with boron nitride. *Journal of Nanoscience and Nanotechnology*, **2003**, 3, 179-83	1.3	11
12	Electronic structure and the field emission mechanism of MgO-coated carbon nanotubes. *New Journal of Physics*, **2003**, 5, 152-152	2.9	20
11	Interatomic potential for vanadium suitable for radiation damage simulations. *Journal of Applied Physics*, **2003**, 93, 3328-3335	2.5	61
10	Orbital hybridization and charge transfer in carbon nanopeapods. *Physical Review Letters*, **2003**, 90, 106402	7.4	66
9	Field emission of carbon nanotubes and electronic structure of carbon nanopeapods. *Current Applied Physics*, **2002**, 2, 57-60	2.6	4
8	Growth and field emission of carbon nanotubes on sodalime glass at 550°C using thermal chemical vapor deposition. *Chemical Physics Letters*, **2001**, 337, 398-402	2.5	50
7	Role of the localized states in field emission of carbon nanotubes. *Physical Review B*, **2000**, 61, 9986-9989	3.3	124

6	Ab initio study on the molecular recognition by metalloporphyrins: CO interaction with iron porphyrin. *Physical Review E*, **1999**, 59, 2218-2221	2.4	11
5	Development of an energy barrier at the metal-chain□metallic-carbon-nanotube nanocontact. *Physical Review B*, **1999**, 60, 6074-6079	3.3	50
4	Wavelets in all-electron density-functional calculations. *Physical Review B*, **1999**, 60, 1437-1440	3.3	18
3	Enhancement of Surface Hardness: Boron on Diamond (111). *Physical Review Letters*, **1998**, 80, 995-998	7.4	18
2	Structural and electronic properties of diamond with hypothetical vacancies stabilized by nitrogen or boron atoms. *Physical Review B*, **1997**, 55, 15349-15352	3.3	9
1	First-Principles Calculations of Luminescence Spectra of Real-Scale Quantum Dots. *ACS Materials Au*,		1