Yong-Chae Chung

List of Publications by Year
in descending order

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141 papers	3,273 citations	172457 29 h-index	168389 53 g-index
142 all docs	142 docs citations	142 times ranked	4768 citing authors

#	Article	IF	Citations
1	Si/Ge Double-Layered Nanotube Array as a Lithium Ion Battery Anode. ACS Nano, 2012, 6, 303-309.	14.6	225
2	Poly(fluorenyl aryl piperidinium) membranes and ionomers for anion exchange membrane fuel cells. Nature Communications, 2021, 12, 2367.	12.8	193
3	Dominant Factors Governing the Rate Capability of a TiO₂ Nanotube Anode for High Power Lithium Ion Batteries. ACS Nano, 2012, 6, 8308-8315.	14.6	184
4	Tunable Indirect to Direct Band Gap Transition of Monolayer Sc₂CO₂ by the Strain Effect. ACS Applied Materials & Interfaces, 2014, 6, 14724-14728.	8.0	175
5	Understanding the anchoring behavior of titanium carbide-based MXenes depending on the functional group in Li S batteries: A density functional theory study. Journal of Power Sources, 2017, 342, 64-69.	7.8	135
6	Achieving Type I, II, and III Heterojunctions Using Functionalized MXene. ACS Applied Materials & Interfaces, 2015, 7, 7163-7169.	8.0	120
7	Modulating magnetic characteristics of Pt embedded graphene by gas adsorption (N2, O2, NO2, SO2). Applied Surface Science, 2014, 289, 445-449.	6.1	103
8	Photocatalytic Activity of Ni 8 wt%-Doped TiO2 Photocatalyst Synthesized by Mechanical Alloying Under Visible Light. Journal of the American Ceramic Society, 2006, 89, 515-518.	3.8	87
9	Role of Multivalent Pr in the Formation and Migration of Oxygen Vacancy in Pr-Doped Ceria: Experimental and First-Principles Investigations. Chemistry of Materials, 2012, 24, 4261-4267.	6.7	86
10	Flexible highly-effective energy harvester via crystallographic and computational control of nanointerfacial morphotropic piezoelectric thin film. Nano Research, 2017, 10, 437-455.	10.4	86
11	Achieving a direct band gap in oxygen functionalized-monolayer scandium carbide by applying an electric field. Physical Chemistry Chemical Physics, 2014, 16, 26273-26278.	2.8	82
12	Electronically Doubleâ€Layered Metal Boride Hollow Nanoprism as an Excellent and Robust Water Oxidation Electrocatalysts. Advanced Energy Materials, 2019, 9, 1803799.	19.5	74
13	Facile preparation of large aspect ratio ellipsoidal anatase TiO2 nanoparticles and their application to dye-sensitized solar cell. Electrochemistry Communications, 2009, 11, 909-912.	4.7	73
14	Hydrogen adsorption on Li metal in boron-substituted graphene: An ab initio approach. International Journal of Hydrogen Energy, 2010, 35, 3583-3587.	7.1	70
15	Effect of nitrogen induced defects in Li dispersed graphene onÂhydrogen storage. International Journal of Hydrogen Energy, 2013, 38, 4611-4617.	7.1	59
16	Functionalized Sulfide Solid Electrolyte with Air-Stable and Chemical-Resistant Oxysulfide Nanolayer for All-Solid-State Batteries. ACS Omega, 2020, 5, 26015-26022.	3.5	58
17	Effect of lithium-trapping on nitrogen-doped graphene as an anchoring material for lithiumâ€“sulfur batteries: a density functional theory study. Physical Chemistry Chemical Physics, 2017, 19, 28189-28194.	2.8	56
18	Non-uniformly functionalized titanium carbide-based MXenes as an anchoring material for Li-S batteries: A first-principles calculation. Applied Surface Science, 2018, 435, 210-215.	6.1	51

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19	Hydrogen storage in Li dispersed graphene with Stoneâ€“Wales defects: A first-principles study. International Journal of Hydrogen Energy, 2014, 39, 13189-13194.	7.1	50
20	Greatly improved electrochemical performance of lithiumâ€“oxygen batteries with a bimetallic platinumâ€“copper alloy catalyst. Journal of Power Sources, 2015, 288, 296-301.	7.8	49
21	Surface alloy formation of Co on Al surface: Molecular dynamics simulation. Journal of Applied Physics, 2003, 93, 8564-8566.	2.5	47
22	Boosting oxygen evolution reaction of transition metal layered double hydroxide by metalloid incorporation. Nano Energy, 2020, 75, 104945.	16.0	47
23	Effective catalytic media using graphitic nitrogen-doped site in graphene for a non-aqueous Liâ€“O2 battery: A density functional theory study. Journal of Power Sources, 2015, 277, 222-227.	7.8	44
24	Carbon-free and two-dimensional cathode structure based on silicene for lithiumâ€“oxygen batteries: A first-principles calculation. Journal of Power Sources, 2015, 275, 32-37.	7.8	37
25	Comparative study of metal atom adsorption on free-standing h-BN and h-BN/Ni (111) surfaces. Applied Surface Science, 2014, 299, 29-34.	6.1	36
26	Electronic structure and half-metallic property of Mn-doped Î²-SiC diluted magnetic semiconductor. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2006, 126, 194-196.	3.5	34
27	Stress evolution during the oxidation of silicon nanowires in the sub-10 nm diameter regime. Applied Physics Letters, 2011, 99, .	3.3	33
28	Structural stability and electronic properties of multi-functionalized two-dimensional chromium carbides. Thin Solid Films, 2016, 619, 131-136.	1.8	33
29	Effect of N-cyclic cationic groups in poly(phenylene oxide)-based catalyst ionomer membranes for anion exchange membrane fuel cells. Journal of Membrane Science, 2020, 608, 118183.	8.2	32
30	Hydrogen storage in Al and Ti dispersed on graphene with boron substitution: First-principles calculations. Computational Materials Science, 2010, 49, S297-S301.	3.0	29
31	Enhanced hydrogen storage properties under external electric fields of N-doped graphene with Li decoration. Physical Chemistry Chemical Physics, 2013, 15, 3243.	2.8	29
32	Atomic-level investigation of interface structure in Niâ€“Al multilayer system: molecular dynamics simulation. Journal of Magnetism and Magnetic Materials, 2005, 286, 394-398.	2.3	27
33	Surface characteristics of epitaxially grown Ni layers on Al surfaces: Molecular dynamics simulation. Journal of Applied Physics, 2006, 100, 074905.	2.5	25
34	Performance characteristics of micro single-chamber solid oxide fuel cell: Computational analysis. Journal of Power Sources, 2006, 154, 35-41.	7.8	25
35	Bandgap engineering of graphene by corrugation on lattice-mismatched MgO (111). Journal of Materials Chemistry C, 2013, 1, 1595.	5.5	25
36	Lattice distortion effect on electrical properties of GDC thin films: Experimental evidence and computational simulation. Solid State Ionics, 2012, 229, 45-53.	2.7	24

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37	Lattice-strain effect on oxygen vacancy formation in gadolinium-doped ceria. Journal of Electroceramics, 2014, 32, 72-77.	2.0	24
38	Polarized Electronic Configuration in Transition Metalâ€“Fluoride Oxide Hollow Nanoprism for Highly Efficient and Robust Water Splitting. ACS Applied Energy Materials, 2019, 2, 3999-4007.	5.1	24
39	The Influence of Cu and Au on Field Aided Lateral Crystallization of Amorphous Silicon Films. Japanese Journal of Applied Physics, 2000, 39, 6191-6195.	1.5	20
40	Molecular dynamics simulation of nano-scale Feâ€“Al thin film growth. Materials Letters, 2006, 60, 1063-1067.	2.6	20
41	Lithium Adsorption on Hexagonal Boron Nitride Nanosheet Using Dispersion-Corrected Density Functional Theory Calculations. Japanese Journal of Applied Physics, 2013, 52, 06GG08.	1.5	20
42	Heterostructural phase diagram of Ga2O3â€“based solid solution with Al2O3. Journal of the European Ceramic Society, 2021, 41, 611-616.	5.7	19
43	Atomic-level investigation of Al and Ni thin film growth on Ni(111) surface: Molecular dynamics simulation. Applied Surface Science, 2007, 253, 8896-8900.	6.1	18
44	Cathode reaction mechanism on the h-BN/Ni (111) heterostructure for the lithium-oxygen battery. Journal of Power Sources, 2016, 307, 379-384.	7.8	18
45	Ferroelectric control of magnetic anisotropy of FePt/BaTiO3 magnetoelectric heterojunction: A density functional theory study. Journal of Applied Physics, 2013, 113, .	2.5	17
46	Theoretical Approach toward Optimum Anion-Doping on MXene Catalysts for Hydrogen Evolution Reaction: an Ab Initio Thermodynamics Study. ACS Applied Materials & Interfaces, 2021, 13, 37035-37043.	8.0	17
47	Calculation of the contribution to grain boundary diffusion in ionic systems that arises from enhanced defect concentrations adjacent to the boundary. Journal of Applied Physics, 2000, 87, 2747-2752.	2.5	16
48	Characterization of Ru layer for capping/buffer application in EUVL mask. Microelectronic Engineering, 2006, 83, 688-691.	2.4	16
49	Asymmetric surface intermixing during thin-film growth in the Coâ€“Al system: Role of local acceleration of the deposited atoms. Acta Materialia, 2008, 56, 1011-1017.	7.9	16
50	Magnetic and half-metallic properties of Cr-doped /spl beta/-SiC. IEEE Transactions on Magnetics, 2005, 41, 2733-2735.	2.1	15
51	Electronic Properties of Transitionâ€Metalâ€Decorated Silicene. ChemPhysChem, 2014, 15, 4095-4099.	2.1	15
52	First-Principles Calculations of Atomistic Behaviors in Ni/Al (001) and Al/Ni (001) System. Japanese Journal of Applied Physics, 2005, 44, 5700-5702.	1.5	14
53	The electronic structure of Ni doped rutile TiO2. Journal of Electroceramics, 2006, 17, 951-953.	2.0	14
54	Metal (Li, Al, Ca and Ti) Absorbed Graphene with Defects for Hydrogen Storage: First-Principles Calculations. Journal of Nanoscience and Nanotechnology, 2011, 11, 10624-10628.	0.9	14

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55	Strain effects on hydrogen storage in Ti decorated pyridinic N-doped graphene. Physical Chemistry Chemical Physics, 2013, 15, 12757.	2.8	14
56	Computer simulation of the resonance characteristics and the sensitivity of cantilever-shaped Al/PZT/RuO2 biosensor. Sensors and Actuators B: Chemical, 2004, 97, 98-102.	7.8	13
57	Molecular dynamics investigation of interfacial mixing behavior in transition metals (Fe, Co, Ni)-Al multilayer system. Journal of Applied Physics, 2009, 105, 034902.	2.5	13
58	Effects of suboxide layers on the electronic properties of Si(100)/SiO2 interfaces: Atomistic multi-scale approach. Journal of Applied Physics, 2013, 113, .	2.5	13
59	Functionalization effect on a Pt/carbon nanotube composite catalyst: a first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 22687-22692.	2.8	13
60	Atomic Mixing Behavior of Co/Al(001) vs. Al/fcc-Co(001): Molecular Dynamics Simulation. Journal of Electroceramics, 2004, 13, 315-320.	2.0	12
61	Atomic Investigation of Al/Ni(001) by Molecular Dynamics Simulation. Japanese Journal of Applied Physics, 2006, 45, 99-101.	1.5	12
62	Defect-induced semiconductor to metal transition in graphene monoxide. Physical Chemistry Chemical Physics, 2014, 16, 13477-13482.	2.8	12
63	Novel absorber stack for minimizing shadow effect in extreme ultraviolet mask. Journal of Vacuum Science & Technology B, 2006, 24, 2820.	1.3	11
64	The early stage of deposition process for Feâ€“Cu magnetic multilayer systems: molecular dynamics simulation. Journal Physics D: Applied Physics, 2009, 42, 135305.	2.8	11
65	Effects of interfacial bonding in the Si-carbon nanotube nanocomposite: A molecular dynamics approach. Journal of Applied Physics, 2012, 112, .	2.5	11
66	Geometric and magnetic properties of Co adatom decorated nitrogen-doped graphene. Journal of Applied Physics, 2013, 113, .	2.5	11
67	Electric field as a novel switch for magnetization of Fe/graphene system. Journal of Magnetism and Magnetic Materials, 2014, 362, 93-96.	2.3	11
68	Numerical modeling of micro single-chamber ceria-based SOFC. Journal of Electroceramics, 2006, 17, 959-964.	2.0	10
69	A Comparative Study of Catalytic Partial Oxidation of Methane Over Ceo₂ Supported Metallic Catalysts. Journal of Nanoscience and Nanotechnology, 2011, 11, 6414-6419.	0.9	10
70	Work function tuning of an ultrathin MgO film on an Ag substrate by generating oxygen impurities at the interface. Thin Solid Films, 2013, 544, 541-544.	1.8	10
71	Graphene Monoxide Bilayer As a High-Performance on/off Switching Media for Nanoelectronics. ACS Applied Materials & Interfaces, 2016, 8, 10477-10482.	8.0	10
72	Elucidating the unintentional p-type nature of spinel Co3O4: A defect study using ab-initio calculation. Journal of the European Ceramic Society, 2018, 38, 629-635.	5.7	10

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73	Effects of B-site substitution on the surface adsorption properties and catalytic activities of La0.8Sr0.2(Mn1â^'xCox)O3. Applied Catalysis A: General, 2010, 387, 203-208.	4.3	9
74	Spin-polarized bandgap of graphene induced by alternative chemisorption with MgO (1 1 1) substrate. Carbon, 2014, 77, 208-214.	10.3	9
75	Theoretical calculations on atomistic behaviors in transition metals (Fe, Co, Ni)â€“Al multilayer system: ab initio approach. Applied Surface Science, 2006, 252, 8380-8383.	6.1	8
76	Interface-Dependent Spin-Reorientation Energy Barrier in Fe/MgO(001) Thin Film. IEEE Electron Device Letters, 2011, 32, 1287-1289.	3.9	8
77	Theoretical dopant screening and processing optimization for vanadium disulfide as cathode material for Li-air batteries: A density functional theory study. Applied Surface Science, 2020, 508, 145276.	6.1	8
78	Enhancement of the quantum capacitances of group-14 elemental two-dimensional materials by Ti-doping: A first principles study. Applied Surface Science, 2020, 530, 147301.	6.1	8
79	Molecular dynamics investigation for thin film growth morphology of Ni/Ni(111). IEEE Transactions on Magnetics, 2005, 41, 3431-3433.	2.1	7
80	Surface structures and magnetic anisotropies of a Fe/Pt (001) surface: An ab initio study. Journal of Applied Physics, 2011, 109, 07B764.	2.5	7
81	Nitrogen-tuned bonding mechanism of Li and Ti adatom embedded graphene. Journal of Solid State Chemistry, 2013, 205, 160-164.	2.9	7
82	Assessment of the accuracy of Le Claire's equation for determination of grain boundary diffusion coefficients from solute concentration gradients. Materials Letters, 1996, 28, 47-54.	2.6	6
83	Analysis of Multilayer Structure for Reflection of Extreme-Ultraviolet Wavelength. Japanese Journal of Applied Physics, 2002, 41, 4086-4090.	1.5	6
84	Ab initioInvestigation of the Early Stage of Nano-scale Thin Film Growth: Al and Co Adatoms on Co (111) Surface. Japanese Journal of Applied Physics, 2004, 43, 3815-3817.	1.5	6
85	Surface diffusion and incorporation of adatom in Co/Al (001) system. Journal of Solid State Chemistry, 2005, 178, 47-51.	2.9	6
86	Atomistic behaviors of Co adatom on Al (001) surface: first-principle approach. Journal of Magnetism and Magnetic Materials, 2005, 286, 399-404.	2.3	6
87	Investigation of the initial reactions of lithium oxides on the graphitic carbon nitrides (g-C3N4) for catalyst in non-aqueous lithium - air batteries: A first-principles calculations. Thin Solid Films, 2018, 660, 186-190.	1.8	6
88	Adsorption and Diffusion of Li and Ni on Graphene with Boron Substitution for Hydrogen Storage:Ab-initioMethod. Japanese Journal of Applied Physics, 2011, 50, 06GJ02.	1.5	6
89	Molecular Dynamics Simulation at the Early Stage of Thin-Film Deposition: Al or Co on Co(111). Japanese Journal of Applied Physics, 2004, 43, 3818-3821.	1.5	5
90	First-principles calculations on magnetic properties of interface-rippled Coâ^•Î±-Al2O3â^•Co. Applied Physics Letters, 2006, 88, 132512.	3.3	5

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91	Molecular dynamics simulation of film growth characterization of Fe and Cu on Cu(111) surface in the early stages of the deposition process. Current Applied Physics, 2011, 11, S65-S68.	2.4	5
92	Band engineering in a van der Waals heterostructure using a 2D polar material and a capping layer. Scientific Reports, 2016, 6, 27986.	3.3	5
93	Manipulatable Interface Electric Field and Charge Transfer in a 2D/2D Heterojunction Photocatalyst via Oxygen Intercalation. Catalysts, 2020, 10, 469.	3.5	5
94	Co/CoAl/Co trilayer fabrication using spontaneous intermixing of Co and Al: Molecular dynamics simulation. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2006, 135, 25-29.	3.5	4
95	Atomic-Level Investigation for Surface Characteristics in a Co-Cu Multilayer System: Molecular Dynamics Simulation. IEEE Transactions on Magnetics, 2008, 44, 2903-2906.	2.1	4
96	Atomic-Scale Investigation of the Ti/Al(001) Interface: A Molecular Dynamics Simulation. Japanese Journal of Applied Physics, 2010, 49, 06GJ14.	1.5	4
97	First-principles calculation and luminescence property of Eux:Si5Al1â^'xO1+xN7â^'x green phosphor. Computational Materials Science, 2010, 49, S359-S363.	3.0	4
98	Surface diffusion coefficient determination by uniaxial tensile strain in Pb/Cu(111) surface systems. Current Applied Physics, 2011, 11, S400-S403.	2.4	4
99	Interfacial reaction-dominated full oxidation of 5â€‰nm diameter silicon nanowires. Journal of Applied Physics, 2012, 112, .	2.5	4
100	Oxygen transport in epitaxial La0.875Sr0.125CoO3-Î´ thin-film cathodes for solid oxide fuel cells: Roles of anisotropic strain. Scripta Materialia, 2016, 115, 141-144.	5.2	4
101	Defect structures of sodium and chloride co-substituted hydroxyapatite and its osseointegration capacity. Journal of Materials Science, 2021, 56, 5493-5508.	3.7	4
102	Angular dependency of off-axis illumination on 100-nm-width pattern printability for extreme ultraviolet lithography: Ru/Mo/Si reflector system. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 2004, 22, 2984.	1.6	3
103	Interfacial mixing behavior of Fe-Al magnetic thin films: molecular dynamics Simulation. IEEE Transactions on Magnetics, 2005, 41, 3706-3708.	2.1	3
104	Numerical modeling of absorber characteristics for EUVL. , 2006, 6151, 553.		3
105	Experimental and Simulation Study to Identify Current-Confined Path in Cuâ€“Al Space Layer for CPP-GMR Spin-Valve Applications. IEEE Transactions on Magnetics, 2006, 42, 2633-2635.	2.1	3
106	Energetics of Pb heterostructures formation on the Cu (111) in the early stage of the deposition process. Journal of Applied Physics, 2010, 107, 114315.	2.5	3
107	Atomic structures and behaviors of a fcc Cu(111) surface with submonolayer Pb coverage. Computational Materials Science, 2010, 47, 693-697.	3.0	3
108	Strain-Controllable Magnetism in Co Decorated Pyridinic N-Doped Graphene. IEEE Transactions on Magnetics, 2014, 50, 1-4.	2.1	3

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109	Ab initio Study of the Si Adsorption on Mo(110). Journal of Electroceramics, 2004, 13, 327-330.	2.0	2
110	Ab initio investigations on atomistic behaviors and magnetic properties in Feâ€“Cu multilayer system. Journal of Applied Physics, 2007, 101, 09D119.	2.5	2
111	Adsorption and Diffusion of Li and Ni on Graphene with Boron Substitution for Hydrogen Storage: Ab-initio Method. Japanese Journal of Applied Physics, 2011, 50, 06GJ02.	1.5	2
112	Surface structure effect on the magnetic anisotropy of Co/Pd (001) thin film: A first principles study. Thin Solid Films, 2015, 589, 252-257.	1.8	2
113	Growth of Nickel Oxide Single Crystals and Bicrystals via hemical Vapor Transport. Journal of the American Ceramic Society, 1996, 79, 695-699.	3.8	1
114	Magnetic property calculations for B2-Co/sub x/Al/sub 1-x/ structures at the interface of Co-Al multilayer. IEEE Transactions on Magnetics, 2005, 41, 3343-3345.	2.1	1
115	Magnetic Anisotropy Variation of Fe Single Atom on Ti/Al(001) Surface by the Change of Ti-Al Surface Phase. Journal of Nanoscience and Nanotechnology, 2011, 11, 6364-6367.	0.9	1
116	Atomic-Scale Investigation on the Ti/Fe(001) Interface Structure: Molecular Dynamics Simulations andAb initioCalculations. Japanese Journal of Applied Physics, 2011, 50, 01BE07.	1.5	1
117	First-principles study on the atomic and electronic structures of graphene-protected magnetic Fe/Ni(111) thin film. Current Applied Physics, 2012, 12, S37-S40.	2.4	1
118	Stable Surface Structures and Magnetic Properties of L1₀-Ordered CoPt Thin Films According to Thin Film Layer Thickness. Journal of Nanoscience and Nanotechnology, 2013, 13, 6316-6320.	0.9	1
119	Fabrication and Characterization of NiO Bicrystals. Materials Research Society Symposia Proceedings, 1994, 357, 139.	0.1	0
120	Analysis of multilayer structure for reflection of extreme ultra-violet wavelength. , 0, , .		0
121	Structural characterization of Mo/Ru/Si EUV reflector by optical modeling. , 0, , .		0
122	Optimization of Low-Energy Electron Beam Proximity Lithography Stencil Mask Structure Factors by Monte Carlo Simulation. Japanese Journal of Applied Physics, 2004, 43, 1196-1198.	1.5	0
123	Numerical investigation of defect printability in extreme ultraviolet (EUV) reflector: Ru/Mo/Si mulitlayer system. , 2004, , .		0
124	Characteristics of Mo/Ru/Si multilayer reflector structure. , 2004, , .		0
125	Atomistic investigations of alpha-Fe thin film growth on Al [100]. , 2004, , .		0
126	First-principles calculations of the atomistic behaviors in Ni/Al [001] and Al/Ni [001] system. , 2004, , .		0

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127	Molecular dynamics investigations for thin film growth morphology of Ni/Ni(111). , 2005, , .		0
128	Electronic structure and magnetic property of Mn adsorbed /spl beta/-SiC(100). , 2005, , .		0
129	Magnetic property calculations for B2-Co/sub x/Al/sub 1-x/ structure at the interface of Co/Al multilayer. , 2005, , .		0
130	Electronic and structural characteristics of atomic diffusion in Fe/Al [001] and Al/Fe [001] systems. , 2005, , .		0
131	Electronic structures and atomic surface diffusion in Cr/Fe(001) and Fe/Cr(001) systems: First-principles study. , 2007, , .		0
132	Surface properties for hydrogen, carbon, and oxygen adsorption on the Ga-terminated (0001) GaN surface system with nitrogen vacancy. , 2007, , .		0
133	Electronic structures of nitrogen doped single walled carbon nanotubes with uniaxial strain: Ab initio method approach. , 2007, , .		0
134	Theoretical investigation of pattern printability of oxidized Si and Ru capping models for extreme ultraviolet lithography (EUVL). Microelectronic Engineering, 2007, 84, 1023-1026.	2.4	0
135	Ab initio investigation of interfacial layer formation in the Moâ^•Si boundary for extreme ultraviolet lithography. Journal of Applied Physics, 2008, 103, 124310.	2.5	0
136	Structural effect of LaAlO<inf>3</inf>/SrTiO<inf>3</inf> interface on electronic properties: Ab-initio calculations. , 2010, , .		0
137	Strain-induced Wurtzite to h-BN Phase Transformation in Zinc Oxide nanorods. , 2010, , .		0
138	Hydrogen adsorption on Li metal in boron substituted graphene: ab initio approach. , 2010, , .		0
139	Electronic Structures and Magnetism of Al/Fe(001) Thin-Film Systems: First-Principles Calculations. Japanese Journal of Applied Physics, 2011, 50, 01BF03.	1.5	0
140	Atomic-Scale Investigation on the Ti/Fe(001) Interface Structure: Molecular Dynamics Simulations andAb initioCalculations. Japanese Journal of Applied Physics, 2011, 50, 01BE07.	1.5	0
141	Electronic Structures and Magnetism of Al/Fe(001) Thin-Film Systems: First-Principles Calculations. Japanese Journal of Applied Physics, 2011, 50, 01BF03.	1.5	0