Gyeong S Hwang

List of Publications by Year
in descending order

148 papers	6,442 citations	87888 38 h-index	69250 77 g-index
152 all docs	152 docs citations	152 times ranked	9305 citing authors

#	Article	IF	Citations
1	An experimental/computational study of steric hindrance effects on <scp>CO₂</scp> absorption in (non)aqueous amine solutions. AICHE Journal, 2022, 68, .	3.6	10
2	Facile Carbamic Acid Intermediate Formation in Aqueous Monoethanolamine and Its Vital Role in CO₂ Capture Processes. Industrial & Engineering Chemistry Research, 2022, 61, 4475-4479.	3.7	11
3	Combined experimental and computational study on the promising monoethanolamineÂ+Â2-(ethylamino)ethanolÂ+Âsulfolane biphasic aqueous solution for CO2 absorption. Chemical Engineering Journal, 2022, 446, 136674.	12.7	11
4	First-principles prediction on antimony-doping effects on the cyclic stability of tin anodes for lithium-ion batteries. Physical Chemistry Chemical Physics, 2022, 24, 17542-17546.	2.8	1
5	Intriguing Thermal Degradation Behavior of Aqueous Piperazine for Carbon Dioxide Capture: A First-Principles Assessment. ACS Sustainable Chemistry and Engineering, 2022, 10, 9584-9590.	6.7	4
6	Dissociative chemisorption of methyl fluoride and its implications for atomic layer etching of silicon nitride. Applied Surface Science, 2021, 543, 148557.	6.1	10
7	Agent molecule modulated low-temperature activation of solid-state lithium-ion transport for polymer electrolytes. Journal of Power Sources, 2021, 505, 229917.	7.8	4
8	Fundamentals of Capacitive Charge Storage in Carbon-Based Supercapacitors. Springer Series in Materials Science, 2021, , 559-586.	0.6	0
9	First-Principles Assessment of Anomalous Thermal Degradation of Aqueous 2-Amino-2-methyl-1-propanol for CO₂ Capture. Energy & Fuels, 2021, 35, 16705-16712.	5.1	7
10	On the mechanism of predominant urea formation from thermal degradation of CO₂-loaded aqueous ethylenediamine. Physical Chemistry Chemical Physics, 2020, 22, 17336-17343.	2.8	12
11	First-Principles Mechanistic Study of the Initial Growth of SrO by Atomic Layer Deposition on TiO2-Terminated SrTiO3 (001). Journal of Physical Chemistry C, 2020, 124, 28116-28122.	3.1	3
12	Anomalous Facile Carbamate Formation at High Stripping Temperatures from Carbon Dioxide Reaction with 2-Amino-2-methyl-1-propanol in Aqueous Solution. ACS Sustainable Chemistry and Engineering, 2020, 8, 18671-18677.	6.7	10
13	First-principles description of electrocatalytic characteristics of graphene-like materials. Journal of Chemical Physics, 2020, 153, 214704.	3.0	2
14	Partial oxidation of methane to methanol by isolated Pt catalyst supported on a CeO2 nanoparticle. Journal of Chemical Physics, 2020, 152, 054715.	3.0	14
15	Interaction of oxygen with polystyrene and polyethylene polymer films: A mechanistic study. Journal of Applied Physics, 2020, 127, .	2.5	20
16	Kinetic Selectivity of Lithium Alkyl Carbonate Formation from Combination Reactions of Ethylene Carbonate Radical Anions. Journal of Physical Chemistry C, 2020, 124, 25754-25759.	3.1	1
17	Theoretical Prediction of the Strong Solvent Effect on Reduced Ethylene Carbonate Ring-Opening and Its Impact on Solid Electrolyte Interphase Evolution. Journal of Physical Chemistry C, 2019, 123, 17695-17702.	3.1	11
18	Psesudocubic Phase Tungsten Oxide as a Photocatalyst for Hydrogen Evolution Reaction. ACS Applied Energy Materials, 2019, 2, 8792-8800.	5.1	19

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19	Freestanding 1T MoS₂/graphene heterostructures as a highly efficient electrocatalyst for lithium polysulfides in Liâ€“S batteries. Energy and Environmental Science, 2019, 12, 344-350.	30.8	510
20	Toward a Reversible Calciumâ€Sulfur Battery with a Lithiumâ€Ion Mediation Approach. Advanced Energy Materials, 2019, 9, 1803794.	19.5	43
21	Strong thermal conductivity dependence on arsenic-vacancy complex formation in arsenic-doped silicon. Journal of Applied Physics, 2019, 126, 195104.	2.5	1
22	Molecular dynamics investigation of reduced ethylene carbonate aggregation at the onset of solid electrolyte interphase formation. Physical Chemistry Chemical Physics, 2019, 21, 22449-22455.	2.8	5
23	Molecular mechanisms for thermal degradation of CO₂-loaded aqueous monoethanolamine solution: a first-principles study. Physical Chemistry Chemical Physics, 2019, 21, 22132-22139.	2.8	22
24	Theoretical evaluation of ethylene carbonate anion transport and its impact on solid electrolyte interphase formation. Electrochimica Acta, 2018, 266, 326-331.	5.2	9
25	Theoretical evaluation of thermal decomposition of dichlorosilane for plasma-enhanced atomic layer deposition of silicon nitride: the important role of surface hydrogen. Physical Chemistry Chemical Physics, 2018, 20, 29152-29158.	2.8	9
26	Fundamental Understanding of CO₂ Capture and Regeneration in Aqueous Amines from First-Principles Studies: Recent Progress and Remaining Challenges. Industrial & Engineering Chemistry Research, 2017, 56, 6887-6899.	3.7	70
27	Molecular dynamics investigation of the thermal conductivity of ternary siliconâ€“germaniumâ€“tin alloys. Journal Physics D: Applied Physics, 2017, 50, 494001.	2.8	12
28	Understanding CO2 capture mechanisms in aqueous hydrazine via combined NMR and first-principles studies. Physical Chemistry Chemical Physics, 2017, 19, 24067-24075.	2.8	12
29	Controlling Plasmonâ€Enhanced Fluorescence via Intersystem Crossing in Photoswitchable Molecules. Small, 2017, 13, 1701763.	10.0	15
30	Molecular insights into the enhanced rate of CO2 absorption to produce bicarbonate in aqueous 2-amino-2-methyl-1-propanol. Physical Chemistry Chemical Physics, 2017, 19, 32116-32124.	2.8	16
31	Silicon-based anode materials for lithium-ion batteries. Series in Materials Science and Engineering, 2017, , 443-460.	0.1	0
32	Plasmonic Nanostructures: Controlling Plasmonâ€Enhanced Fluorescence via Intersystem Crossing in Photoswitchable Molecules (Small 38/2017). Small, 2017, 13, .	10.0	0
33	What is the thermal conductivity limit of silicon germanium alloys?. Physical Chemistry Chemical Physics, 2016, 18, 19544-19548.	2.8	18
34	Molecular Insights into the Complex Relationship between Capacitance and Pore Morphology in Nanoporous Carbon-based Supercapacitors. ACS Applied Materials & Interfaces, 2016, 8, 34659-34667.	8.0	19
35	Theoretical Analysis of Thermal Transport in Graphene Supported on Hexagonal Boron Nitride: The Importance of Strong Adhesion Due to<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Ï€</mml:mi></mml:math>-Bond Polarization. Physical Review Applied, 2016, 6, .	3.8	23
36	Structure and Li⁺ ion transport in a mixed carbonate/LiPF₆ electrolyte near graphite electrode surfaces: a molecular dynamics study. Physical Chemistry Chemical Physics, 2016, 18, 27868-27876.	2.8	39

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37	Recent progress in first-principles simulations of anode materials and interfaces for lithium ion batteries. Current Opinion in Chemical Engineering, 2016, 13, 75-81.	7.8	9
38	First-principles assessment of CO₂ capture mechanisms in aqueous piperazine solution. Physical Chemistry Chemical Physics, 2016, 18, 25296-25307.	2.8	26
39	The Bright Future for Electrode Materials of Energy Devices: Highly Conductive Porous Na-Embedded Carbon. Nano Letters, 2016, 16, 8029-8033.	9.1	50
40	Charging Rate Dependence of Ion Migration and Stagnation in Ionic-Liquid-Filled Carbon Nanopores. Journal of Physical Chemistry C, 2016, 120, 24560-24567.	3.1	35
41	Materials science of Ru and Ru alloy thin films for barrier applications. , 2016, , .		0
42	On the Importance of Regulating Hydroxyl Coverage on the Basal Plane of Graphene Oxide for Supercapacitors. ChemElectroChem, 2016, 3, 741-748.	3.4	6
43	Highâ€Performance Lithiumâ€Sulfur Batteries with a Selfâ€Supported, 3D Li₂Sâ€Doped Graphene Aerogel Cathodes. Advanced Energy Materials, 2016, 6, 1501355.	19.5	183
44	Importance of Pd monomer pairs in enhancing the oxygen reduction reaction activity of the AuPd(1 0) Tj ETQq0 0 0 rgBT /Overlock 10 T	4.4	14
45	Ultrafast chemical lithiation of single crystalline silicon nanowires: in situ characterization and first principles modeling. RSC Advances, 2015, 5, 17438-17443.	3.6	11
46	On the influence of polarization effects in predicting the interfacial structure and capacitance of graphene-like electrodes in ionic liquids. Journal of Chemical Physics, 2015, 142, 024701.	3.0	44
47	Role of different Pd/Pt ensembles in determining CO chemisorption on Au-based bimetallic alloys: A first-principles study. Applied Surface Science, 2015, 332, 409-418.	6.1	4
48	Anomalous Stagewise Lithiation of Gold-Coated Silicon Nanowires: A Combined In Situ Characterization and First-Principles Study. ACS Applied Materials & Interfaces, 2015, 7, 16976-16983.	8.0	9
49	Long-life Li/polysulphide batteries with high sulphur loading enabled by lightweight three-dimensional nitrogen/sulphur-codoped graphene sponge. Nature Communications, 2015, 6, 7760.	12.8	923
50	A Comparative First-Principles Study on Sodiation of Silicon, Germanium, and Tin for Sodium-Ion Batteries. Journal of Physical Chemistry C, 2015, 119, 14843-14850.	3.1	95
51	On the origin of preferred bicarbonate production from carbon dioxide (CO₂) capture in aqueous 2-amino-2-methyl-1-propanol (AMP). Physical Chemistry Chemical Physics, 2015, 17, 29184-29192.	2.8	38
52	Electron small polarons and their transport in bismuth vanadate: a first principles study. Physical Chemistry Chemical Physics, 2015, 17, 256-260.	2.8	81
53	Reaction mechanisms of aqueous monoethanolamine with carbon dioxide: a combined quantum chemical and molecular dynamics study. Physical Chemistry Chemical Physics, 2015, 17, 831-839.	2.8	95
54	Formation, nature, and stability of the arsenic-silicon-oxygen alloy for plasma doping of non-planar silicon structures. Applied Physics Letters, 2014, 105, 262102.	3.3	3

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55	Fundamental insight into control of thermal conductivity in silicon-germanium alloy nanowires. Materials Research Society Symposia Proceedings, 2014, 1707, 31.	0.1	0
56	On the origin of the significant difference in lithiation behavior between silicon and germanium. Journal of Power Sources, 2014, 263, 252-258.	7.8	44
57	Tailoring the performance of graphene-based supercapacitors using topological defects: A theoretical assessment. Carbon, 2014, 68, 734-741.	10.3	78
58	Synergetic Role of Photogenerated Electrons and Holes in the Oxidation of CO to CO₂ on Reduced TiO₂(110): A First-Principles Study. ACS Catalysis, 2014, 4, 4051-4056.	11.2	20
59	On the origin of anisotropic lithiation in crystalline silicon over germanium: A first principles study. Applied Surface Science, 2014, 323, 78-81.	6.1	14
60	Impact of Graphene Edges on Enhancing the Performance of Electrochemical Double Layer Capacitors. Journal of Physical Chemistry C, 2014, 118, 21770-21777.	3.1	54
61	Magnetoâ€convection in a rotating layer of nanofluid. Asia-Pacific Journal of Chemical Engineering, 2014, 9, 663-677.	1.5	50
62	Large Capacitance Enhancement Induced by Metal-Doping in Graphene-Based Supercapacitors: A First-Principles-Based Assessment. ACS Applied Materials & Interfaces, 2014, 6, 12168-12176.	8.0	40
63	Nanocolumnar Germanium Thin Films as a High-Rate Sodium-Ion Battery Anode Material. Journal of Physical Chemistry C, 2013, 117, 18885-18890.	3.1	175
64	Curvature Effects on the Interfacial Capacitance of Carbon Nanotubes in an Ionic Liquid. Journal of Physical Chemistry C, 2013, 117, 23539-23546.	3.1	53
65	A computational analysis of graphene adhesion on amorphous silica. Journal of Applied Physics, 2013, 113, 164901.	2.5	19
66	Lithiation Behavior of Silicon-Rich Oxide (SiO_{1/3}): A First-Principles Study. Chemistry of Materials, 2013, 25, 3435-3440.	6.7	80
67	Relative contributions of quantum and double layer capacitance to the supercapacitor performance of carbon nanotubes in an ionic liquid. Physical Chemistry Chemical Physics, 2013, 15, 19741-19747.	2.8	68
68	Role of the surfaceâ€“subsurface interlayer interaction in enhancing oxygen hydrogenation to water in Pd3Co alloy catalysts. Physical Chemistry Chemical Physics, 2013, 15, 12118.	2.8	9
69	On the Origin of the Enhanced Supercapacitor Performance of Nitrogen-Doped Graphene. Journal of Physical Chemistry C, 2013, 117, 5610-5616.	3.1	230
70	A Computational Study of the Interfacial Structure and Capacitance of Graphene in [BMIM][PF₆] Ionic Liquid. Journal of the Electrochemical Society, 2013, 160, A1-A10.	2.9	229
71	Structural phase-dependent hole localization and transport in bismuth vanadate. Physical Review B, 2013, 87, .	3.2	71
72	Communication: Enhanced oxygen reduction reaction and its underlying mechanism in Pd-Ir-Co trimetallic alloys. Journal of Chemical Physics, 2013, 139, 201104.	3.0	37

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73	Microsegregation effects on the thermal conductivity of silicon-germanium alloys. Journal of Applied Physics, 2013, 114, 174910.	2.5	12
74	Role of Small Pd Ensembles in Boosting CO Oxidation in AuPd Alloys. Journal of Physical Chemistry Letters, 2012, 3, 566-570.	4.6	40
75	Mechanism of thermal conductivity suppression in doped silicon studied with nonequilibrium molecular dynamics. Physical Review B, 2012, 86, .	3.2	30
76	Large Thermoelectric Figure-of-Merits from SiGe Nanowires by Simultaneously Measuring Electrical and Thermal Transport Properties. Nano Letters, 2012, 12, 2918-2923.	9.1	181
77	Hybrid density functional study of the structural, bonding, and electronic properties of bismuth vanadate. Physical Review B, 2012, 86, .	3.2	55
78	Force-matching-based parameterization of the Stillinger-Weber potential for thermal conduction in silicon. Physical Review B, 2012, 85, .	3.2	37
79	Atomic Arrangements in AuPt/Pt(100) and AuPd/Pd(100) Surface Alloys: A Monte Carlo Study Using First Principles-Based Cluster Expansions. Journal of Physical Chemistry C, 2011, 115, 21205-21210.	3.1	9
80	A Comparative First-Principles Study of the Structure, Energetics, and Properties of Liâ€“M (M = Si, Ge,) Tj ETQq0 0 0 rgBT /Overlock 10	3.1	125
81	Structure and Properties of Liâ^'Si Alloys: A First-Principles Study. Journal of Physical Chemistry C, 2011, 115, 2514-2521.	3.1	187
82	Effects of vacancy defects on thermal conductivity in crystalline silicon: A nonequilibrium molecular dynamics study. Physical Review B, 2011, 83, .	3.2	65
83	Atomistic structural description of the Si(001)/a-SiO₂interface: The influence of different Keating-like potential parameters. Journal of Applied Physics, 2011, 109, 113519.	2.5	10
84	Factors in the Metal Doping of BiVO₄ for Improved Photoelectrocatalytic Activity as Studied by Scanning Electrochemical Microscopy and First-Principles Density-Functional Calculation. Journal of Physical Chemistry C, 2011, 115, 17870-17879.	3.1	409
85	Defectâ€Assisted Covalent Binding of Graphene to an Amorphous Silica Surface: A Theoretical Prediction. ChemPhysChem, 2011, 12, 2155-2159.	2.1	2
86	Pd ensemble effects on oxygen hydrogenation in AuPd alloys: A combined density functional theory and Monte Carlo study. Catalysis Today, 2011, 165, 138-144.	4.4	34
87	Structure and energetics of amorphous SiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow		

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91	Geometric Parameter Effects on Ensemble Contributions to Catalysis: H₂O₂ Formation from H₂ and O₂ on AuPd Alloys. A First Principles Study. Journal of Physical Chemistry C, 2010, 114, 14922-14928.	3.1	56
92	First-principles study of the mechanical and optical properties of amorphous hydrogenated silicon and silicon-rich silicon oxide. Physical Review B, 2010, 81, .	3.2	24
93	On the Nature and Behavior of Li Atoms in Si: A First Principles Study. Journal of Physical Chemistry C, 2010, 114, 17942-17946.	3.1	82
94	On the Nature and Origin of Si Surface Segregation in Amorphous AuSi Alloys. Journal of Physical Chemistry C, 2010, 114, 3037-3041.	3.1	17
95	Atomic Arrangements of AuPt/Pt(111) and AuPd/Pd(111) Surface Alloys: A Combined Density Functional Theory and Monte Carlo Study. Journal of Physical Chemistry C, 2010, 114, 21516-21523.	3.1	24
96	Biaxial strain effects on the structure and stability of self-interstitial clusters in silicon. Physical Review B, 2009, 79, .	3.2	9
97	Formation and structure of vacancy defects in silicon: Combined Metropolis Monte Carlo, tight-binding molecular dynamics, and density functional theory calculations. Physical Review B, 2009, 80, .	3.2	8
98	Theoretical characterization of silicon self-interstitial clusters in uniform strain fields. Physical Review B, 2009, 80, .	3.2	8
99	Prediction of the formation of stable periodic self-interstitial cluster chains [(I4)m,m=1â€“4] in Si under biaxial strain. Applied Physics Letters, 2009, 94, 264101.	3.3	8
100	Arsenic defect complexes atSiO2/Siinterfaces: A density functional theory study. Physical Review B, 2009, 80, .	3.2	2
101	Epoxide reduction with hydrazine on graphene: A first principles study. Journal of Chemical Physics, 2009, 131, 064704.	3.0	151
102	Integrated atomistic modelling of interstitial defect growth in silicon. Molecular Simulation, 2009, 35, 867-879.	2.0	7
103	On the Role of Pd Ensembles in Selective H₂O₂ Formation on PdAu Alloys. Journal of Physical Chemistry C, 2009, 113, 12943-12945.	3.1	125
104	Strain-Induced Formation of Surface Defects in Amorphous Silica: A Theoretical Prediction. Physical Review Letters, 2008, 100, 076104.	7.8	21
105	Theoretical determination of stable fourfold coordinated vacancy clusters in silicon. Physical Review B, 2008, 78, .	3.2	18
106	Interstitial-based boron diffusion dynamics in amorphous silicon. Applied Physics Letters, 2008, 93, .	3.3	3
107	Structure and stability of small compact self-interstitial clusters in crystalline silicon. Physical Review B, 2008, 77, .	3.2	34
108	Effects of P on amorphous chemical vapor deposition Ru-P alloy films for Cu interconnect liner applications. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2008, 26, 974-979.	2.1	17

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109	Growth and shape transition of small silicon self-interstitial clusters. Physical Review B, 2008, 78, .	3.2	27
110	Structure, energetics, and bonding of amorphous Auâ€“Si alloys. Journal of Chemical Physics, 2007, 127, 224710.	3.0	27
111	An Experimental and Simulation Study of Arsenic Diffusion Behavior in Point Defect Engineered Silicon. Materials Research Society Symposia Proceedings, 2007, 994, 1.	0.1	0
112	Chemical Routes to Ultra Thin Films for Copper Barriers and Liners. Materials Research Society Symposia Proceedings, 2007, 990, 1.	0.1	0
113	On the origin of Si nanocrystal formation in a Si suboxide matrix. Journal of Applied Physics, 2007, 102, .	2.5	41
114	Structure of small Aun, Agn, and Cun clusters (n=2â^'4) on rutile TiO2(110): A density functional theory study. Computational and Theoretical Chemistry, 2006, 771, 129-133.	1.5	31
115	Structure and Interconversion of Oxygen-Vacancy-Related Defects on Amorphous Silica. Physical Review Letters, 2006, 97, 066101.	7.8	23
116	O2-coverage-dependent CO oxidation on reduced TiO2(110): A first principles study. Journal of Chemical Physics, 2006, 125, 144706.	3.0	34
117	Understanding of the Synthesis and Structure of Si Nanocrystals in an Oxide Matrix from First Principles Based Atomistic Modeling. Materials Research Society Symposia Proceedings, 2006, 958, 1.	0.1	0
118	Ab-Initio Study of Boron Diffusion Retardation in Si1-xGex. Materials Research Society Symposia Proceedings, 2006, 912, 1.	0.1	0
119	Interstitial-Mediated Arsenic Clustering in Ultrashallow Junction Formation. Electrochemical and Solid-State Letters, 2006, 9, G354.	2.2	21
120	Multiscale Modeling of Growth and Structure of Silicon Nanoparticles in an Oxide Matrix. Materials Research Society Symposia Proceedings, 2006, 978, .	0.1	0
121	Mechanisms for Interstitial-Mediated Transient Enhanced Diffusion of N-type Dopants. Materials Research Society Symposia Proceedings, 2006, 912, 1.	0.1	0
122	Interstitial-mediated mechanisms of As and P diffusion in Si: Gradient-corrected density-functional calculations. Physical Review B, 2006, 74, .	3.2	13
123	Nucleation and growth of 1B metal clusters on rutile TiO2(110): Atomic level understanding from first principles studies. Catalysis Today, 2005, 105, 78-84.	4.4	22
124	Origin of nonlocal interactions in adsorption of polar molecules on Si(001)-2Ã—1. Journal of Chemical Physics, 2005, 122, 164706.	3.0	26
125	Silicon interstitials atSiâ•SiO2interfaces: Density functional calculations. Physical Review B, 2005, 72, .	3.2	24
126	Growth and structure of small gold particles on rutileTiO2(110). Physical Review B, 2005, 72, .	3.2	62

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127	Structure and dynamics of the diarsenic complex in crystalline silicon. Physical Review B, 2005, 72, .	3.2	9
128	Diffusion of Fluorine-Silicon Interstitial Complex in Crystalline Silicon. Materials Research Society Symposia Proceedings, 2005, 864, 911.	0.1	0
129	Role of Interstitials in As TED and Clustering in Crystalline Silicon. Materials Research Society Symposia Proceedings, 2005, 864, 851.	0.1	0
130	Tunnel oxide thickness dependence of activation energy for SiGe quantum dot flash memory. , 2005, , .		0
131	Structure, stability, and diffusion of arsenic-silicon interstitial pairs. Applied Physics Letters, 2005, 87, 231905.	3.3	26
132	Boron diffusion in strained Si:â€ƒA first-principles study. Journal of Applied Physics, 2004, 96, 5543-5547.	2.5	8
133	Interaction of neutral vacancies and interstitials with theSi(001)surface. Physical Review B, 2004, 70, .	3.2	13
134	Dynamics of oxygen species on reducedTiO2(110)rutile. Physical Review B, 2004, 70, .	3.2	60
135	Behavior of Si Interstitials and Boron-Interstitial Pairs at the Si/SiO2 Interface. Materials Research Society Symposia Proceedings, 2004, 810, 398.	0.1	0
136	A comparative theoretical study of Au, Ag and Cu adsorption on TiO2 (110) rutile surfaces. Korean Journal of Chemical Engineering, 2004, 21, 537-547.	2.7	20
137	Surface chemistry effects on vacancy and interstitial annihilation on Si(001). Physica Status Solidi (B): Basic Research, 2004, 241, 2303-2312.	1.5	9
138	Revisit to the Ising model for orderâ€“disorder phase transition on Si(001). Surface Science, 2004, 554, 150-158.	1.9	7
139	Mechanisms of monovacancy annihilation and type-A defect creation on Si(001)â€“2Ã—1. Surface Science, 2004, 555, 187-192.	1.9	7
140	Two-dimensional arrangement of CH3NH2 adsorption on Si(0 0 1)-2 Ã— 1. Chemical Physics Letters, 2004, 385, 144-148.	2.6	8
141	Effects of Subsurface Boron and Phosphorus on Surface Reactivity of Si(001):Â Water and Ammonia Adsorption. Journal of Physical Chemistry B, 2004, 108, 16147-16153.	2.6	3
142	Function of subsurface boron on Si(001)-2Ã—1: water adsorption. Surface Science, 2003, 547, L882-L886.	1.9	6
143	Adsorption of Au atoms on stoichiometric and reduced TiO2(110) rutile surfaces: a first principles study. Surface Science, 2003, 542, 72-80.	1.9	87
144	Catalytic role of boron atoms in self-interstitial clustering in Si. Applied Physics Letters, 2003, 83, 1047-1049.	3.3	12

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145	Shouldering in B diffusion profiles in Si: Role of di-boron diffusion. Applied Physics Letters, 2003, 83, 3501-3503.	3.3	9
146	Diffusion of the Diboron Pair in Silicon. Physical Review Letters, 2002, 89, 055901.	7.8	14
147	Diffusion and dissociation of neutral divacancies in crystalline silicon. Physical Review B, 2002, 65, .	3.2	39
148	A channel for dimer flipping on the Si(001) surface. Surface Science, 2000, 465, L789-L793.	1.9	27