Noboru Takeuchi

List of Publications by Year
in descending order

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140	2,822	159585	214800
papers	citations	30 h-index	47 g-index

141	141	141	2203
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Antiferromagnetic coupling in the initial stages of the MnN epitaxial growth on the CrN (0 0 1) surface. Applied Surface Science, 2022, 573, 151451.	6.1	7
2	Self-energy corrected band-gap tuning induced by strain in the hexagonal boron phosphide monolayer. Computational Materials Science, 2022, 203, 111144.	3.0	7
3	Controlling the magnetic alignment at the MnGa/Co2MnSi interface: A DFT study. Journal of Magnetism and Magnetic Materials, 2022, 547, 168936.	2.3	3
4	An atomistic study on the structural and thermodynamic properties of Alâ€“Fe bimetallic nanoparticles during melting and solidification: The role of size and composition. Materials Chemistry and Physics, 2022, 282, 125936.	4.0	5
5	Understanding the Selectivity of the Oxygen Reduction Reaction at the Atomistic Level on Nitrogenâ€Doped Graphitic Carbon Materials. Advanced Energy Materials, 2021, 11, 2002459.	19.5	63
6	A first-principles study of the atomic layer deposition of ZnO on carboxyl functionalized carbon nanotubes: the role of water molecules. Physical Chemistry Chemical Physics, 2021, 23, 3467-3478.	2.8	5
7	Understanding the Noncollinear Antiferromagnetic IrMn3 Surfaces and Their Exchange-Biased Heterostructures from First-Principles. ACS Applied Electronic Materials, 2021, 3, 1086-1096.	4.3	3
8	Adsorption of crotonaldehyde on metal surfaces: Cu vs Pt. Journal of Chemical Physics, 2021, 154, 104701.	3.0	10
9	Surface structures of magnetostrictive D03-Fe3Ga(0Â0Â1). Applied Surface Science, 2021, 553, 149488.	6.1	5
10	Investigating the magnetic and atomic interface configuration for a model Fe/CrN bilayer system. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2021, 39, 063209.	2.1	3
11	Role of oligomer structures in the surface chemistry of amidinate metal complexes used for atomic layer deposition of thin films. Journal of Materials Research, 2020, 35, 720-731.	2.6	7
12	Formaldehyde adsorption on a hydrogenated gallium nitride monolayer: A density functional theory study. Applied Surface Science, 2020, 506, 144944.	6.1	13
13	Exchange bias and exchange spring effects in Fe/CrN bilayers. Journal Physics D: Applied Physics, 2020, 53, 125001.	2.8	13
14	Structural, electronic, and magnetic properties of the CoGa (0â€¯0â€¯1) surface and the L10 MnGa/CoGa interface: A density functional theory study. Applied Surface Science, 2020, 504, 144332.	6.1	3
15	Adsorption and diffusion mechanisms of silver ad-atoms on Ag and Cu (110) surfaces: A first principles study. Materials Today Communications, 2020, 25, 101461.	1.9	4
16	Structural properties and thermal stability of multi-walled black phosphorene nanotubes and their operation as temperature driven nanorotors. Nanoscale, 2020, 12, 18313-18321.	5.6	6
17	Understanding the first half-ALD cycle of the ZnO growth on hydroxyl functionalized carbon nanotubes. Physical Chemistry Chemical Physics, 2020, 22, 15333-15339.	2.8	3
18	Aldehyde trapping by self-propagating atom-exchange reactions on a gallium nitride monolayer: role of the molecule complexity. New Journal of Chemistry, 2020, 44, 12843-12849.	2.8	6

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19	Density Functional Theory Study of the Adsorption and Dissociation of Copper(I) Acetamidinates on Ni(110): The Effect of the Substrate. Journal of Physical Chemistry C, 2020, 124, 15366-15376.	3.1	5
20	Kinetic Study of the Hydrogenation of Unsaturated Aldehydes Promoted by CuPt_x/SBA-15 Single-Atom Alloy (SAA) Catalysts. ACS Catalysis, 2020, 10, 3431-3443.	11.2	53
21	Coadsorption of Formic Acid and Hydrazine on Cu(110) Single-Crystal Surfaces. Journal of Physical Chemistry C, 2019, 123, 7584-7593.	3.1	16
22	Puckered arsenene single-walled nanotubes: Stability, geometry, and electronic properties. Computational Materials Science, 2019, 169, 109108.	3.0	5
23	Controlling Selectivity in Unsaturated Aldehyde Hydrogenation Using Single-Site Alloy Catalysts. ACS Catalysis, 2019, 9, 9150-9157.	11.2	55
24	N-Doped carbon nanotubes enriched with graphitic nitrogen in a buckypaper configuration as efficient 3D electrodes for oxygen reduction to H₂O₂. Nanoscale, 2019, 11, 2829-2839.	5.6	54
25	Nitrogen-induced reconstructions on the Cr(001) surface. Applied Surface Science, 2019, 484, 578-586.	6.1	0
26	Formaldehyde adsorption on a hydrogenated aluminum nitride monolayer: A self-propagated reaction. Computational and Theoretical Chemistry, 2019, 1159, 18-22.	2.5	8
27	Functionalization of silicene and silicane with benzaldehyde. Journal of Molecular Modeling, 2019, 25, 109.	1.8	8
28	Formaldehyde trapping by radical initiated reaction on hydrogenated boron nitride. Applied Surface Science, 2019, 484, 470-478.	6.1	12
29	Density Functional Theory Study of the Surface Adsorption and Dissociation of Copper(I) Acetamidinates on Cu(110) Surfaces. Journal of Physical Chemistry C, 2019, 123, 4341-4348.	3.1	12
30	Silicene as an efficient way to fully inactivate the SO2 pollutant. Applied Surface Science, 2019, 479, 847-851.	6.1	11
31	Structural transition induced by compression and stretching of puckered arsenene nanotubes. Physical Chemistry Chemical Physics, 2019, 21, 22467-22474.	2.8	6
32	Zig-zag boron nitride nanotubes functionalization with acetylene molecules: a density functional theory study. Adsorption, 2019, 25, 63-74.	3.0	4
33	DFT study of the dimethyl sulfoxide reduction on silicene. Applied Surface Science, 2019, 467-468, 261-267.	6.1	7
34	Formation of ferromagnetic/ferrimagnetic epitaxial interfaces: Stability and magnetic properties. Computational Materials Science, 2018, 144, 294-303.	3.0	10
35	Mn induced 1â€Ã—â€2 reconstruction in the Ï„-MnAl(0â€0â€1) surface. Journal of Crystal Growth, 2018, 489, 24-30.	1.8	0
36	Structural, electronic, and magnetic properties of the CrN (0â€0â€1) surface: First-principles studies. Applied Surface Science, 2018, 454, 350-357.	6.1	21

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37	Zinc-blende MnN bilayer formation on the GaN(111) surface. Superlattices and Microstructures, 2017, 107, 189-196.	3.1	7
38	Structural, electronic and magnetic properties of the MnGa(111)-1 Ã— 2 and 2 Ã— 2 reconstructions: Spin polarized first principles total energy calculations. Applied Surface Science, 2017, 419, 286-293.	6.1	3
39	Structural stability and the electronic and magnetic properties of ferrimagnetic Mn 4 N(0 0 1) surfaces. Applied Surface Science, 2017, 407, 209-212.	6.1	8
40	Structural and magnetic phase transitions in chromium nitride thin films grown by rf nitrogen plasma molecular beam epitaxy. Physical Review B, 2017, 96, .	3.2	28
41	Formaldehyde adsorption on graphane. Computational and Theoretical Chemistry, 2017, 1117, 119-123.	2.5	14
42	Acetylene chain reaction on hydrogenated boron nitride monolayers: a density functional theory study. Journal of Molecular Modeling, 2017, 23, 359.	1.8	5
43	Organic functionalization of silicane with formaldehyde and propanaldehyde. Applied Surface Science, 2017, 392, 841-848.	6.1	11
44	Ab-initio study of the Y adsorption and YN formation on the GaN(000<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 477 Td (xmlns:m Diffusion pathways and stability. Superlattices and Microstructures, 2016, 96, 67-74.	3.1	4
45	Antiferromagnetic MnN layer on the MnGa(001) surface. Applied Surface Science, 2016, 390, 328-332.	6.1	11
46	Two-dimensional boron nitride structures functionalization: first principles studies. Journal of Molecular Modeling, 2016, 22, 226.	1.8	11
47	Van der Waals molecular interactions in the organic functionalization of graphane, silicane, and germanane with alkene and alkyne molecules: a DFT-D2 study. Journal of Molecular Modeling, 2016, 22, 175.	1.8	9
48	Mn Adsorption on the GaAs(111)â€“(2Ã—2)B Surface: First Principles Studies. Zeitschrift Fur Physikalische Chemie, 2016, 230, 943-954.	2.8	6
49	Nitrogen induced phosphorene formation on the boron phosphide (111) surface: a density functional theory study. RSC Advances, 2016, 6, 108621-108626.	3.6	2
50	Surface reactivity of Ge[111] for organic functionalization by means of a radical-initiated reaction: A DFT study. Applied Surface Science, 2016, 379, 14-22.	6.1	4
51	Formation of InN atomic-size wires by simple N adsorption on the In/Si(111)â€“(4 Ã— 1) surface. Applied Surface Science, 2016, 385, 318-323.	6.1	3
52	Understanding the stability of Fe incorporation within Mn3N2(001) surfaces: An ab-initio study. Applied Surface Science, 2016, 363, 651-658.	6.1	3
53	YN nanostructure formation on the GaN(0001) surface: First principles studies. Computational Materials Science, 2015, 106, 155-160.	3.0	6
54	Structural, electronic and magnetic properties of Mn3N2(0 0 1) surfaces. Applied Surface Science, 2015, 355, 623-630.	6.1	17

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55	Interface formation for a ferromagnetic/antiferromagnetic bilayer system studied by scanning tunneling microscopy and first-principles theory. Physical Review B, 2015, 91, .	3.2	13
56	Adsorption of Organic Molecules on the Hydrogenated Germanene: A DFT Study. Journal of Physical Chemistry C, 2015, 119, 27995-28004.	3.1	23
57	Graphene monolayers on GaN(0001). Applied Surface Science, 2015, 326, 7-11.	6.1	12
58	Iron on GaN(0001) pseudo-1â€‰Ã—â€‰1 (1+112) investigated by scanning tunneling microscopy and first-principles theory. Applied Physics Letters, 2014, 104, 171607.	3.3	3
59	Initial stages of the adsorption of Sc and ScN thin films on GaN(0001): First principles calculations. Applied Surface Science, 2013, 268, 16-21.	6.1	10
60	Density Functional Theory Study of the Organic Functionalization of Hydrogenated Graphene. Journal of Physical Chemistry C, 2013, 117, 18738-18745.	3.1	25
61	Ab-initio studies of the Sc adsorption and the ScN thin film formation on the GaN(000-1)-(2Ã—2) surface. Thin Solid Films, 2013, 548, 317-322.	1.8	8
62	Adsorption, diffusion, and incorporation of Pd in cubic (001) Cu3N: A DFT study. Journal of Alloys and Compounds, 2013, 576, 285-290.	5.5	10
63	Density functional theory study of the organic functionalization of hydrogenated silicene. Journal of Chemical Physics, 2013, 138, 194702.	3.0	38
64	Heteroepitaxial growth and surface structure of L1-MnGa(111) ultra-thin films on GaN(0001). Applied Physics Letters, 2013, 103, .	3.3	15
65	First principles calculations of the Sc adsorption on Si(001)-c(2Ã—4). Surface Science, 2012, 606, 1382-1386.	1.9	8
66	Ab-initio studies of the adsorption of a B ad-atom on GaN surfaces. Journal of Crystal Growth, 2012, 338, 62-68.	1.5	4
67	Cooperative Chiral Adsorption of Styrene Molecules on the Si(001)-c(2 Ã— 4) Surface: First-Principles Investigation of Reaction Mechanisms. Journal of Physical Chemistry C, 2011, 115, 14213-14218.	3.1	2
68	Two-dimensional Mn structure on the GaN growth surface and evidence for room-temperature spin ordering. Physical Review B, 2011, 83, .	3.2	21
69	Ab initio calculations of non-stoichiometric copper nitride, pure and with palladium. Journal of Alloys and Compounds, 2011, 509, 1471-1476.	5.5	19
70	Initial stages of the growth of Al on GaN(0001). Journal of Crystal Growth, 2010, 312, 2419-2422.	1.5	7
71	Ab initio study of the adsorption of antimony and arsenic on the Si(110) surface. Thin Solid Films, 2010, 519, 265-269.	1.8	3
72	Surface Radical Chain Reaction Revisited: Comparative Investigation of Styrene and 2,4-Dimethyl-Styrene on Hydrogenated Si(001) Surface from Density Functional Theory Calculations. Journal of Physical Chemistry C, 2010, 114, 3981-3986.	3.1	22

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73	Toward accurate reaction energetics for molecular line growth at surface: Quantum Monte Carlo and density functional theory calculations. Journal of Chemical Physics, 2009, 131, 214708.	3.0	16
74	First principles total energy calculations of the structural and electronic properties of YGe2 in AlB2 type structures. Solid State Sciences, 2009, 11, 265-270.	3.2	1
75	Structural properties of the formation of yttrium germanides thin films on the Si(111) surface. Thin Solid Films, 2009, 517, 4336-4340.	1.8	0
76	First principles calculations of the adsorption and diffusion of Y on the Si(001)-c(4Ã—2) surface. Surface Science, 2009, 603, 3414-3419.	1.9	4
77	First principles total energy calculations of the surface atomic structure of yttrium disilicide on Si(111). Surface Science, 2008, 602, 644-649.	1.9	8
78	First-principles calculations of the atomic and electronic properties of group IIIA disilicides in AlB2 type structures. Solid State Sciences, 2008, 10, 355-361.	3.2	6
79	Density functional study of the structural properties of silver halides: LDA vs GGA calculations. Solid State Sciences, 2008, 10, 1228-1235.	3.2	31
80	First-principles studies of the surface reaction of acetylene withHâˆ’Si(001)(1Ã—1). Physical Review B, 2007, 75, .	3.2	9
81	First principles calculations of the structural properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Sc</mml:mi><mml:msub><mml:mi mathvariant="normal">Si</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>and the formation of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Sc</mml:mi><mml:msub><mml:mi mathvariant="normal">Si</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>/C60	3.2	7
82	First-principles calculations of the structural and electronic properties of Cu3MN compounds with M=Ni, Cu, Zn, Pd, Ag, and Cd. Solid State Sciences, 2007, 9, 166-172.	3.2	63
83	First principles calculations of the adsorption of acetylene on the Si(001) surface at low and full coverage. Surface Science, 2007, 601, 3361-3365.	1.9	11
84	Adsorption ofSb4on Ge(001) and Si(001) surfaces: Scanning tunneling microscopy and first-principles calculations. Physical Review B, 2006, 73, .	3.2	8
85	First principles total energy studies of the adsorption of germane on Ge(001)-c(2Ã—4). Thin Solid Films, 2005, 490, 196-200.	1.8	6
86	Density Functional Theory Study of One-Dimensional Growth of Styrene on the Hydrogen-Terminated Si(001)â˜(3 Ã— 1) Surface. Journal of Physical Chemistry B, 2005, 109, 11967-11972.	2.6	31
87	Role of Molecular Conjugation in the Surface Radical Reaction of Aldehydes with Hâˆ’Si(111):â€‰ First Principles Study. Journal of Physical Chemistry B, 2005, 109, 18889-18894.	2.6	31
88	Adsorption and diffusion of Ga and N adatoms on GaN surfaces: Comparing the effects of Ga coverage and electronic excitation. Physical Review B, 2005, 72, .	3.2	42
89	Ab initio total energy calculations of copper nitride: the effect of lattice parameters and Cu content in the electronic properties. Solid State Sciences, 2004, 6, 9-14.	3.2	88
90	Theoretical study of the stability of wurtzite, zinc-blende, NaCl and CsCl phases in group IIIB and IIIA nitrides. Physica Status Solidi (B): Basic Research, 2004, 241, 2424-2428.	1.5	31

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91	Surface Reaction of Alkynes and Alkenes with H-Si(111):Â A Density Functional Theory Study. Journal of the American Chemical Society, 2004, 126, 15890-15896.	13.7	86
92	First principles total energy calculations of the adsorption of germane and digermane on Si(001)-c(2Ã—4). Surface Science, 2003, 547, 9-18.	1.9	3
93	A molecule of H2S on the Si(001)c(2Ã—4) surface: a first principles calculation. Surface Science, 2003, 524, 157-163.	1.9	6
94	First principles calculations of the local arrangement of silicon hydrides on the Si()-c(2Ã—4) surface. Surface Science, 2003, 529, 274-280.	1.9	10
95	First principles total energy calculations of the structural and electronic properties of ScxGa1â€“xN. Physica Status Solidi (B): Basic Research, 2003, 238, 127-135.	1.5	40
96	First principles total energy calculations of the adsorption of single Cl2 and Br2 molecules on the Si(001)-c(2Ã— 4) surface. Physica Status Solidi (B): Basic Research, 2003, 239, 345-352.	1.5	4
97	First principles calculations of the ground state properties and structural phase transformation in YN. Journal of Physics Condensed Matter, 2003, 15, 2625-2633.	1.8	54
98	Surface properties of YN(001):â€ƒA first-principles calculation. Physical Review B, 2002, 66, .	3.2	49
99	First-principles calculations of the structural and electronic properties of the ScN(001) surface. Physical Review B, 2002, 65, .	3.2	40
100	Atomic structure of the indium-inducedGe(001)(nÃ—4)surface reconstruction determined by scanning tunneling microscopy andab initiocalculations. Physical Review B, 2002, 66, .	3.2	5
101	THE LOW COVERAGE PHASES OF Pb ON Ge(001): SCANNING TUNNELING MICROSCOPY AND FIRST PRINCIPLES. Surface Review and Letters, 2002, 09, 1809-1814.	1.1	0
102	S ON Si(001): ADSORPTION OF A SINGLE ATOM UP TO A FULL MONOLAYER. Surface Review and Letters, 2002, 09, 1815-1819.	1.1	2
103	First-principles calculations of the ground-state properties and stability of ScN. Physical Review B, 2002, 65, .	3.2	140
104	First principles calculations of the ground-state properties and structural phase transformation in CdO. Physical Review B, 2002, 66, .	3.2	84
105	First principles total energy calculations of the Al induced Si(001)-(3Ã—4) reconstruction. Surface Science, 2002, 504, 101-107.	1.9	11
106	First principles total energy calculations of the adsorption of Cl, Cl2, and HCl on Ge-c(2Ã—4). Surface Science, 2002, 521, 95-103.	1.9	12
107	First principles calculations of the adsorption of single group III and group V atoms on Si(0 0 1). Surface Science, 2001, 482-485, 44-48.	1.9	6
108	Bond conserving rotation, adatoms and rest atoms in the reconstruction of Si() and Ge() surfaces: a first principles study. Surface Science, 2001, 494, 21-27.	1.9	19

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109	First-principles calculations of the atomic structure of the In-inducedSi(001)â˜(4Ã—3)reconstruction. Physical Review B, 2001, 63, .	3.2	28
110	First-principles calculations of the adsorption of a single monolayer of GaAs on Si(110). Physical Review B, 2001, 64, .	3.2	4
111	First-principles calculations of the adsorption of S on theSi(001)c(4Ã—2)surface. Physical Review B, 2001, 64, .	3.2	3
112	Scanning tunneling microscopy andab initiocalculations:c(4Ã—8)reconstructions of Pb on Si and Ge(001). Physical Review B, 2001, 64, .	3.2	10
113	First-principles calculations of theSi(110)(2Ã—3)Sbsurface. Physical Review B, 2000, 61, 16704-16707.	3.2	12
114	Atomic structure of the low-coverage(2Ã—2)phases of Al, Ga, and In on Ge(001). Physical Review B, 2000, 61, 9925-9927.	3.2	12
115	First-principles calculations of the growth of InSb on GaSb(110). Physical Review B, 2000, 61, 15581-15584.	3.2	2
116	Adsorption of group III and group V metals on Si(001): One-dimensional versus two-dimensional growth. Physical Review B, 2000, 63, .	3.2	43
117	Role of missing rows in the adsorption of Te on Si(001). Physical Review B, 1999, 60, 4796-4799.	3.2	14
118	Tellurium on Ge(001): a perfect restoration of the (1Ã—1) symmetry?. Surface Science, 1999, 426, L433-L439.	1.9	13
119	Defects and energy barriers in the Si(100)â€“Sb and Si(100)â€“As surfaces: a theoretical study. Surface Science, 1999, 432, 239-244.	1.9	11
120	First-principles calculations of theSi(111)â˜c(2Ã—8)surface. Physical Review B, 1998, 57, 6255-6257.	3.2	10
121	First principles calculations of the different structures of a monolayer of Sb on Si (111). Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1998, 16, 1790-1793.	2.1	15
122	Stability of thec(4Ã—8)structure in the adsorption of Pb in the (100) surface of elemental semiconductors. Physical Review B, 1998, 58, R7504-R7507.	3.2	13
123	First-principles calculations of the initial growth of Pb on Si(100). Physical Review B, 1998, 58, 16172-16176.	3.2	36
124	Symmetric Sb dimers and the possibility of mixed Si-Ge layers in the Sb/Ge/Si(100) surface. Physical Review B, 1997, 56, 7446-7448.	3.2	15
125	Symmetric dimers on the Ge(100)-2Ã—1-Sb surface. Physical Review B, 1997, 55, 2417-2419.	3.2	34
126	Ab initio molecular dynamics study of amorphous Ge. Solid State Communications, 1996, 98, 591-594.	1.9	9

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127	Firstâ€principles calculations of the atomic and electronic structure of the Sbâ€“Ge(111)(2Ã—1) surface. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1996, 14, 1652-1655.	2.1	5
128	Structure determination of a Sb monolayer on Ge(111) from first-principles calculations. Physical Review B, 1996, 53, 7996-8000.	3.2	15
129	Atomic dynamics and structure of the Ge(111)c(2Ã—8) surface. Physical Review B, 1995, 51, 10844-10850.	3.2	26
130	Reconstructions and phase transitions at semiconductor surfaces: Ge(111). Surface Science, 1995, 331-333, 995-1001.	1.9	8
131	Metallization and incomplete melting of a semiconductor surface at high temperature. Physical Review Letters, 1994, 72, 2227-2230.	7.8	78
132	Ab initiomolecular-dynamics study of structural, dynamical, and electronic properties of liquid Ge. Physical Review B, 1994, 50, 8342-8347.	3.2	46
133	Adatom diffusion and disordering at the Ge(111)-c(2Ã—8)â€“(1Ã—1) surface transition. Physical Review B, 1994, 49, 10757-10760.	3.2	45
134	Energy barriers, adatom diffusion and field-induced disordering of the Ge(111)c(2 Ã— 8) surface at T â‰ˆ 300Â°C. Surface Science, 1994, 307-309, 755-760.	1.9	11
135	Do we know the true structure of Ge(111)c(2Ã—8)?. Physical Review Letters, 1992, 69, 648-651.	7.8	113
136	Au(111): A theoretical study of the surface reconstruction and the surface electronic structure. Physical Review B, 1991, 43, 13899-13906.	3.2	141
137	Reconstruction of the (100) surfaces of Au and Ag. Physical Review B, 1991, 43, 14363-14370.	3.2	56
138	Structural and electronic properties of the (111)2Ã—1 surface of Ge from first-principles calculations. Physical Review B, 1991, 44, 13611-13617.	3.2	48
139	First-principles calculations of equilibrium ground-state properties of Au and Ag. Physical Review B, 1989, 40, 1565-1570.	3.2	60
140	Theoretical study of noble-metal (100) surface reconstructions using first-principles techniques. Physical Review Letters, 1989, 63, 1273-1276.	7.8	74