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	Au(111): A theoretical study of the surface reconstruction and the surface electronic structure. Physical Review B, 1991, 43, 13899-13906.	3.2	141
2	First-principles calculations of the ground-state properties and stability of ScN. Physical Review B, 2002, 65, .	3.2	140
3	Do we know the true structure of Ge(111)c(2Ã—8)?. Physical Review Letters, 1992, 69, 648-651.	7.8	113
4	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
5	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
6	First principles calculations of the ground-state properties and structural phase transformation in CdO. Physical Review B, 2002, 66, .	3.2	84
7	Metallization and incomplete melting of a semiconductor surface at high temperature. Physical Review Letters, 1994, 72, 2227-2230.	7.8	78
8	Theoretical study of noble-metal (100) surface reconstructions using first-principles techniques. Physical Review Letters, 1989, 63, 1273-1276.	7.8	74
9	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
10	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
11	First-principles calculations of equilibrium ground-state properties of Au and Ag. Physical Review B, 1989, 40, 1565-1570.	3.2	60
12	Reconstruction of the (100) surfaces of Au and Ag. Physical Review B, 1991, 43, 14363-14370.	3.2	56
13	Controlling Selectivity in Unsaturated Aldehyde Hydrogenation Using Single-Site Alloy Catalysts. ACS Catalysis, 2019, 9, 9150-9157.	11.2	55
14	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
15	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
16	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
17	Surface properties of YN(001):â€ƒA first-principles calculation. Physical Review B, 2002, 66, .	3.2	49
18	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

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19	Ab initiomolecular-dynamics study of structural, dynamical, and electronic properties of liquid Ge. Physical Review B, 1994, 50, 8342-8347.	3.2	46
20	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
21	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
22	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
23	First-principles calculations of the structural and electronic properties of the ScN(001) surface. Physical Review B, 2002, 65, .	3.2	40
24	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
25	Density functional theory study of the organic functionalization of hydrogenated silicene. Journal of Chemical Physics, 2013, 138, 194702.	3.0	38
26	First-principles calculations of the initial growth of Pb on Si(100). Physical Review B, 1998, 58, 16172-16176.	3.2	36
27	Symmetric dimers on the Ge(100)-2Ã—1-Sb surface. Physical Review B, 1997, 55, 2417-2419.	3.2	34
28	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
29	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
30	Role of Molecular Conjugation in the Surface Radical Reaction of Aldehydes with Hâ^'Si(111):â€‰ First Principles Study. Journal of Physical Chemistry B, 2005, 109, 18889-18894.	2.6	31
31	Density functional study of the structural properties of silver halides: LDA vs GGA calculations. Solid State Sciences, 2008, 10, 1228-1235.	3.2	31
32	First-principles calculations of the atomic structure of the In-inducedSi(001)â^'(4Ã—3)reconstruction. Physical Review B, 2001, 63, .	3.2	28
33	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
34	Atomic dynamics and structure of the Ge(111)c(2Ã—8) surface. Physical Review B, 1995, 51, 10844-10850.	3.2	26
35	Density Functional Theory Study of the Organic Functionalization of Hydrogenated Graphene. Journal of Physical Chemistry C, 2013, 117, 18738-18745.	3.1	25
36	Adsorption of Organic Molecules on the Hydrogenated Germanene: A DFT Study. Journal of Physical Chemistry C, 2015, 119, 27995-28004.	3.1	23

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37	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
38	Two-dimensional Mn structure on the GaN growth surface and evidence for room-temperature spin ordering. Physical Review B, 2011, 83, .	3.2	21
39	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
40	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
41	Ab initio calculations of non-stoichiometric copper nitride, pure and with palladium. Journal of Alloys and Compounds, 2011, 509, 1471-1476.	5.5	19
42	Structural, electronic and magnetic properties of Mn3N2(0 0 1) surfaces. Applied Surface Science, 2015, 355, 623-630.	6.1	17
43	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
44	Coadsorption of Formic Acid and Hydrazine on Cu(110) Single-Crystal Surfaces. Journal of Physical Chemistry C, 2019, 123, 7584-7593.	3.1	16
45	Structure determination of a Sb monolayer on Ge(111) from first-principles calculations. Physical Review B, 1996, 53, 7996-8000.	3.2	15
46	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
47	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
48	Heteroepitaxial growth and surface structure of L1-MnGa(111) ultra-thin films on GaN(0001). Applied Physics Letters, 2013, 103, .	3.3	15
49	Role of missing rows in the adsorption of Te on Si(001). Physical Review B, 1999, 60, 4796-4799.	3.2	14
50	Formaldehyde adsorption on graphane. Computational and Theoretical Chemistry, 2017, 1117, 119-123.	2.5	14
51	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
52	Tellurium on Ge(001): a perfect restoration of the (1Ã—1) symmetry?. Surface Science, 1999, 426, L433-L439.	1.9	13
53	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
54	Formaldehyde adsorption on a hydrogenated gallium nitride monolayer: A density functional theory study. Applied Surface Science, 2020, 506, 144944.	6.1	13

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55	Exchange bias and exchange spring effects in Fe/CrN bilayers. Journal Physics D: Applied Physics, 2020, 53, 125001.	2.8	13
56	First-principles calculations of theSi(110)(2Ã—3)Sbsurface. Physical Review B, 2000, 61, 16704-16707.	3.2	12
57	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
58	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
59	Graphene monolayers on GaN(0001). Applied Surface Science, 2015, 326, 7-11.	6.1	12
60	Formaldehyde trapping by radical initiated reaction on hydrogenated boron nitride. Applied Surface Science, 2019, 484, 470-478.	6.1	12
61	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
62	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
63	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
64	First principles total energy calculations of the Al induced Si(001)-(3Ã—4) reconstruction. Surface Science, 2002, 504, 101-107.	1.9	11
65	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
66	Antiferromagnetic MnN layer on the MnGa(001) surface. Applied Surface Science, 2016, 390, 328-332.	6.1	11
67	Two-dimensional boron nitride structures functionalization: first principles studies. Journal of Molecular Modeling, 2016, 22, 226.	1.8	11
68	Organic functionalization of silicane with formaldehyde and propanaldehyde. Applied Surface Science, 2017, 392, 841-848.	6.1	11
69	Silicene as an efficient way to fully inactivate the SO2 pollutant. Applied Surface Science, 2019, 479, 847-851.	6.1	11
70	First-principles calculations of theSi(111)â”c(2Ã—8)surface. Physical Review B, 1998, 57, 6255-6257.	3.2	10
71	Scanning tunneling microscopy andab initiocalculations:c(4Ã—8)reconstructions of Pb on Si and Ge(001). Physical Review B, 2001, 64, .	3.2	10
72	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

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73	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
74	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
75	Formation of ferromagnetic/ferrimagnetic epitaxial interfaces: Stability and magnetic properties. Computational Materials Science, 2018, 144, 294-303.	3.0	10
76	Adsorption of crotonaldehyde on metal surfaces: Cu vs Pt. Journal of Chemical Physics, 2021, 154, 104701.	3.0	10
77	Ab initio molecular dynamics study of amorphous Ge. Solid State Communications, 1996, 98, 591-594.	1.9	9
78	First-principles studies of the surface reaction of acetylene withHâˆ’Si(001)(1Ã—1). Physical Review B, 2007, 75, .	3.2	9
79	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
80	Reconstructions and phase transitions at semiconductor surfaces: Ge(111). Surface Science, 1995, 331-333, 995-1001.	1.9	8
81	Adsorption ofSb4on Ge(001) and Si(001) surfaces: Scanning tunneling microscopy and first-principles calculations. Physical Review B, 2006, 73, .	3.2	8
82	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
83	First principles calculations of the Sc adsorption on Si(001)-c(2Ã—4). Surface Science, 2012, 606, 1382-1386.	1.9	8
84	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
85	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
86	Formaldehyde adsorption on a hydrogenated aluminum nitride monolayer: A self-propagated reaction. Computational and Theoretical Chemistry, 2019, 1159, 18-22.	2.5	8
87	Functionalization of silicene and silicane with benzaldehyde. Journal of Molecular Modeling, 2019, 25, 109.	1.8	8
88	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 mathva	3.2	7
89	Initial stages of the growth of Al on GaN(0001). Journal of Crystal Growth, 2010, 312, 2419-2422.	1.5	7
90	Zinc-blende MnN bilayer formation on the GaN(111) surface. Superlattices and Microstructures, 2017, 107, 189-196.	3.1	7

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91	DFT study of the dimethyl sulfoxide reduction on silicene. Applied Surface Science, 2019, 467-468, 261-267.	6.1	7
92	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
93	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
94	Self-energy corrected band-gap tuning induced by strain in the hexagonal boron phosphide monolayer. Computational Materials Science, 2022, 203, 111144.	3.0	7
95	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
96	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
97	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
98	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
99	YN nanostructure formation on the GaN(0001) surface: First principles studies. Computational Materials Science, 2015, 106, 155-160.	3.0	6
100	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
101	Structural transition induced by compression and stretching of puckered arsenene nanotubes. Physical Chemistry Chemical Physics, 2019, 21, 22467-22474.	2.8	6
102	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
103	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
104	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
105	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
106	Acetylene chain reaction on hydrogenated boron nitride monolayers: a density functional theory study. Journal of Molecular Modeling, 2017, 23, 359.	1.8	5
107	Puckered arsenene single-walled nanotubes: Stability, geometry, and electronic properties. Computational Materials Science, 2019, 169, 109108.	3.0	5
108	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

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109	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
110	Surface structures of magnetostrictive D03-Fe3Ga(0Â0Â1). Applied Surface Science, 2021, 553, 149488.	6.1	5
111	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
112	First-principles calculations of the adsorption of a single monolayer of GaAs on Si(110). Physical Review B, 2001, 64, .	3.2	4
113	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
114	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
115	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
116	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
117	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
118	Zig-zag boron nitride nanotubes functionalization with acetylene molecules: a density functional theory study. Adsorption, 2019, 25, 63-74.	3.0	4
119	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
120	First-principles calculations of the adsorption of S on theSi(001)c(4Ã—2)surface. Physical Review B, 2001, 64, .	3.2	3
121	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
122	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
123	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
124	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
125	Understanding the stability of Fe incorporation within Mn3N2(001) surfaces: An ab-initio study. Applied Surface Science, 2016, 363, 651-658.	6.1	3
126	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

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127	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
128	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
129	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
130	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
131	Controlling the magnetic alignment at the MnGa/Co2MnSi interface: A DFT study. Journal of Magnetism and Magnetic Materials, 2022, 547, 168936.	2.3	3
132	First-principles calculations of the growth of InSb on GaSb(110). Physical Review B, 2000, 61, 15581-15584.	3.2	2
133	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
134	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
135	Nitrogen induced phosphorene formation on the boron phosphide (111) surface: a density functional theory study. RSC Advances, 2016, 6, 108621-108626.	3.6	2
136	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
137	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
138	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
139	Mn induced 1â€Ã—â€2 reconstruction in the Ï„-MnAl(0â€0â€1) surface. Journal of Crystal Growth, 2018, 489, 24-30.	1.5	0
140	Nitrogen-induced reconstructions on the Cr(001) surface. Applied Surface Science, 2019, 484, 578-586.	6.1	0