Jun-Hyung Cho

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155 papers	3,393 citations	29 h-index	50 g-index
160 ext. papers	3,815 ext. citations	4.2 avg, IF	5.44 L-index

#	Paper	IF	Citations
155	Multivalency-Driven Formation of Te-Based Monolayer Materials: A Combined First-Principles and Experimental study. *Physical Review Letters*, **2017**, 119, 106101	7.4	285
154	Electronic properties of N- and C-doped TiO2. *Applied Physics Letters*, **2005**, 87, 011904	3.4	199
153	Physisorption of DNA Nucleobases on h-BN and Graphene: vdW-Corrected DFT Calculations. *Journal of Physical Chemistry C*, **2013**, 117, 13435-13441	3.8	163
152	Weakly correlated one-dimensional indium chains on Si(111). *Physical Review B*, **2001**, 64,	3.3	101
151	Assembling phenomena of calix[4]hydroquinone nanotube bundles by one-dimensional short hydrogen bonding and displaced pi-pi stacking. *Journal of the American Chemical Society*, **2002**, 124, 14268-79	16.4	101
150	Flatbands and Emergent Ferromagnetic Ordering in Fe_{3}Sn_{2} Kagome Lattices. *Physical Review Letters*, **2018**, 121, 096401	7.4	94
149	Anomalous doping effect in black phosphorene using first-principles calculations. *Physical Chemistry Chemical Physics*, **2015**, 17, 16351-8	3.6	93
148	Dilute Magnetic Semiconductor and Half-Metal Behaviors in 3d Transition-Metal Doped Black and Blue Phosphorenes: A First-Principles Study. *Nanoscale Research Letters*, **2016**, 11, 77	5	78
147	Adsorption kinetics of acetylene and ethylene on Si(001). *Physical Review B*, **2004**, 69,	3.3	78
146	Surface Relaxation and Ferromagnetism of Rh(001). *Physical Review Letters*, **1997**, 78, 1299-1302	7.4	69
145	Dissociative adsorption of water on the Si(001) surface: A first-principles study. *Physical Review B*, **2000**, 61, 4503-4506	3.3	59
144	Anomalously Large Thermal Expansion at the (0001) Surface of Beryllium without Observable Interlayer Anharmonicity. *Physical Review Letters*, **1998**, 80, 2853-2856	7.4	59
143	Oscillatory lattice relaxation at metal surfaces. *Physical Review B*, **1999**, 59, 1677-1680	3.3	55
142	Adsorption of cyclopentene on the Si(001) surface: A first-principles study. *Physical Review B*, **2001**, 64,	3.3	54
141	One-dimensional molecular wire on hydrogenated Si(001). *Physical Review B*, **2002**, 65,	3.3	50
140	Ab initio pseudopotential study of Fe, Co, and Ni employing the spin-polarized LAPW approach. *Physical Review B*, **1996**, 53, 10685-10689	3.3	49
139	First-principles study of the adsorption of C2H2 and C2H4 on Si(100). *Physical Review B*, **2001**, 63,	3.3	47

138	H18 Carbon: A New Metallic Phase with sp2-sp3 Hybridized Bonding Network. *Scientific Reports*, **2016**, 6, 21879	4.9	46
137	Influence of intermolecular hydrogen bonding on water dissociation at the MgO(001) surface. *Physical Review B*, **2000**, 62, 9981-9984	3.3	41
136	The Nature of Bonding in Bulk Tellurium Composed of One-Dimensional Helical Chains. *Inorganic Chemistry*, **2018**, 57, 5083-5088	5.1	38
135	Electronic structure of one-dimensional indium chains on Si(111). *Physical Review B*, **2005**, 71,	3.3	38
134	Fluorine-induced local magnetic moment in graphene: A hybrid DFT study. *Physical Review B*, **2013**, 87,	3.3	36
133	Atomic structure and energetics of adsorbed water on the NaCl(001) surface. *Physical Review B*, **2004**, 69,	3.3	35
132	Magnetism of the V(001) surface: Contradictory results from pseudopotential and linearized augmented plane-wave calculations. *Physical Review B*, **2001**, 63,	3.3	35
131	Different adsorption structures of pyridine on Si(001) and Ge(001) surfaces. *Journal of Chemical Physics*, **2004**, 120, 8222-5	3.9	34
130	Final-state pseudopotential theory for the Ge 3d core-level shifts on the Ge/Si(100)-(2 x 1) surface. *Physical Review B*, **1994**, 50, 17139-17142	3.3	34
129	Driving force of phase transition in indium nanowires on Si(111). *Physical Review Letters*, **2013**, 110, 116801	7.4	32
128	Microscopic mechanism of room-temperature superconductivity in compressed LaH10. *Physical Review B*, **2019**, 99,	3.3	31
127	Structure and binding energies of unsaturated hydrocarbons on Si(001) and Ge(001). *Journal of Chemical Physics*, **2006**, 124, 024716	3.9	29
126	Competing Gap Opening Mechanisms of Monolayer Graphene and Graphene Nanoribbons on Strong Topological Insulators. *Nano Letters*, **2017**, 17, 4013-4018	11.5	28
125	Atomic structure of the Sb/Si(100)-(2 x 1) surface. *Physical Review B*, **1995**, 51, 5058-5060	3.3	28
124	Benzene adsorbed on Si(001): The role of electron correlation and finite temperature. *Physical Review B*, **2012**, 85,	3.3	27
123	Two dissociation pathways of water and ammonia on the Si(001) surface. *Journal of Physical Chemistry B*, **2006**, 110, 18455-8	3.4	27
122	Ge-Si intermixing at the Ge/Si(001) surface. *Physical Review B*, **2000**, 61, 1688-1691	3.3	26
121	Ultraviolet-visible absorption spectra of N-doped TiO2 film deposited on sapphire. *Journal of Applied Physics*, **2006**, 100, 113534	2.5	24

120	Hydrogen-bonded array of NH2 on the Si(100) surface. *Physical Review B*, **2000**, 62, 1607-1610	3.3	23
119	Origin of contrasting surface core-level shifts at the Be(101$\bar{1}$0) and Mg(101$\bar{1}$0) surfaces. *Physical Review B*, **2000**, 61, 9975-9978	3.3	23
118	Spin-orbit coupling effects on the stability of two competing structures in Pb/Si(111) and Pb/Ge(111). *Physical Review B*, **2016**, 94,	3.3	22
117	Competing magnetic orderings and tunable topological states in two-dimensional hexagonal organometallic lattices. *Physical Review B*, **2016**, 93,	3.3	22
116	Conversion between two binding states of benzene on Si(001). *Physical Review B*, **2005**, 72,	3.3	22
115	Indium-indium pair correlation and surface segregation in InGaAs alloys. *Physical Review Letters*, **2000**, 84, 3654-7	7.4	22
114	Pressure dependence of the superconducting transition temperature of compressed LaH10. *Physical Review B*, **2019**, 100,	3.3	21
113	Quantum size effects in competing charge and spin orderings of dangling bond wires on Si(001). *Physical Review B*, **2009**, 80,	3.3	21
112	Oscillatory energetics of flat Ag films on MgO(001). *Physical Review B*, **2001**, 63,	3.3	21
111	Oscillatory Nonmetal-Metal Transitions of Ultrathin Sb Overlayers on a GaAs(110) Substrate. *Physical Review Letters*, **1998**, 80, 3582-3585	7.4	21
110	Contrasting structural and bonding properties of trimethylamine and dimethylamine adsorbed on Si(001). *Physical Review B*, **2003**, 68,	3.3	20
109	Antiferromagnetic Slater insulator phase of Na$_2$IrO$_3$. *Scientific Reports*, **2014**, 4, 5253	4.9	19
108	Theoretical prediction of heterogeneous molecular wires on the Si(001) surface. *Journal of the American Chemical Society*, **2006**, 128, 3890-1	16.4	19
107	Nature of the Insulating Ground State of the 5d Postperovskite CaIrO3. *Physical Review Letters*, **2015**, 115, 096401	7.4	18
106	Si 2p core-level shifts at the As/Si(001) and Sb/Si(001) surfaces. *Physical Review B*, **1997**, 55, 15464-15466	3.3	18
105	Plane-wave-basis pseudopotential calculations of the surface relaxations of Ti(0001) and Zr(0001). *Physical Review B*, **1997**, 56, 9282-9285	3.3	18
104	Adsorption structure of 1,4-cyclohexadiene on Si(001). *Journal of Chemical Physics*, **2002**, 116, 3800-3804	3.9	18
103	Plane-wave-basis pseudopotential study of the ground-state properties of Ni. *Physical Review B*, **1995**, 52, 9159-9161	3.3	18

102	Stabilization and manipulation of electronically phase-separated ground states in defective indium atom wires on silicon. *Physical Review Letters*, **2014**, 113, 196802	7.4	17
101	Atomic structure of the Ge/Si(100)-(2 x 1) surface. *Physical Review B*, **1994**, 49, 13670-13673	3.3	17
100	Contrasting interedge superexchange interactions of graphene nanoribbons embedded in h-BN and graphane. *Physical Review B*, **2015**, 92,	3.3	16
99	Core-level shifts of low coordination atoms at the W(320) stepped surface. *Physical Review B*, **2001**, 64,	3.3	16
98	Nature of lattice distortion in one-dimensional dangling-bond wires on Si and C. *Physical Review B*, **2002**, 66,	3.3	16
97	Interplay between the spin-selection rule and frontier orbital theory in O2 activation and CO oxidation by single-atom-sized catalysts on TiO2(110). *Physical Chemistry Chemical Physics*, **2016**, 18, 24872-9	3.6	16
96	Growth mechanism of a 1D molecular line across the dimer rows on H-terminated Si(001). *Physical Review Letters*, **2009**, 102, 166102	7.4	15
95	Atomic structure, energetics, and dynamics of topological solitons in indium chains on Si(111) surfaces. *Physical Review Letters*, **2011**, 106, 026801	7.4	15
94	Enhanced stability of 1D molecular lines on the H-terminated Si(001) surface. *Physical Review Letters*, **2007**, 98, 246101	7.4	15
93	Adsorption structure of 2-butyne on Si(100)-(2×1). *Journal of Chemical Physics*, **2003**, 118, 6083-6088	3.9	15
92	Theoretical study of water adsorption on the Ge(100) surface. *Physical Review B*, **2002**, 66,	3.3	15
91	Instability of one-dimensional dangling-bond wires on H-passivated C(001), Si(001), and Ge(001) surfaces. *Surface Science*, **2011**, 605, L13-L15	1.8	14
90	First-principles calculation of the atomic structure of one-dimensional indium chains on Si(111): Convergence to a metastable structure. *Physical Review B*, **2007**, 76,	3.3	14
89	Self-assembled molecular array in methylamine dissociation on Si(001). *Physical Review B*, **2003**, 67,	3.3	14
88	First-principles study of the adsorption and reaction of cyclopentene on Ge(001). *Physical Review B*, **2003**, 67,	3.3	14
87	Dirac fermions in antiferromagnetic FeSn kagome lattices with combined space inversion and time-reversal symmetry. *Physical Review B*, **2020**, 102,	3.3	14
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85	Isotope effect in superconducting lanthanum hydride under high compression. *Physical Review B*, **2020**, 101,	3.3	13

84	Microscopic mechanism of the tunable band gap in potassium-doped few-layer black phosphorus. *Physical Review B*, **2017**, 96,	3.3	13
83	First-principles study of NH3 decomposition on the Si(001) surface. *Physical Review B*, **2004**, 69,	3.3	13
82	Adsorption structure of acetylene on Ge(001): A first-principles study. *Journal of Chemical Physics*, **2003**, 119, 2820-2824	3.9	13
81	Theoretical prediction of Weyl fermions in the paramagnetic electride Y2C. *Physical Review B*, **2019**, 99,	3.3	12
80	Multiband nature of room-temperature superconductivity in LaH10 at high pressure. *Physical Review B*, **2020**, 101,	3.3	12
79	Origin of the metal-insulator transition of indium atom wires on Si(111). *Physical Review B*, **2016**, 93,	3.3	12
78	Antiferromagnetic superexchange mediated by a resonant surface state in Sn/Si(111). *Physical Review B*, **2014**, 90,	3.3	12
77	Band-gap opening in metallic carbon nanotubes adsorbed on H5Si(001). *Applied Physics Letters*, **2006**, 89, 023124	3.4	12
76	Ab initio calculations of the adsorption and reaction of acetonitrile on Si(001). *Journal of Chemical Physics*, **2003**, 119, 6744-6749	3.9	12
75	Two reaction pathways of acetic acid on the Si(001) surface: Density-functional calculations. *Physical Review B*, **2005**, 72,	3.3	12
74	Geometry and core-level shifts of an adsorbed Sb monolayer on GaAs(110). *Physical Review B*, **1998**, 57, 1352-1355	3.3	12
73	Coupling of charge, lattice, orbital, and spin degrees of freedom in charge density waves in 1TTaS2. *Physical Review B*, **2018**, 97,	3.3	11
72	Ferrimagnetic Slater insulator phase of the Sn/Ge(111) surface. *Physical Review Letters*, **2013**, 111, 106403	7.4	11
71	Theoretical study of the reaction of acrylonitrile on Si(001). *Journal of Chemical Physics*, **2004**, 121, 1557-61	3.9	11
70	Hydrogen catalyzed adsorption of alkenes on the diamond (001) surface. *Physical Review B*, **2003**, 68,	3.3	11
69	Ferromagnetic Weyl Fermions in Two-Dimensional Layered Electride Gd_{2}C. *Physical Review Letters*, **2020**, 125, 187203	7.4	11
68	Stacking-sequence-independent band structure and shear exfoliation of two-dimensional electride materials. *Physical Review B*, **2016**, 94,	3.3	11
67	Atomistic mechanisms of van der Waals epitaxy and property optimization of layered materials. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2017**, 7, e1300	7.9	10

66	Contribution of van der Waals interactions to the adsorption energy of C2H2, C2H4, and C6H6 on Si(100). *Chemical Physics Letters*, **2013**, 557, 159-162	2.5	10
65	Antiferromagnetic coupling between two adjacent dangling bonds on Si(001): Total-energy and force calculations. *Physical Review B*, **2008**, 78,	3.3	10
64	Dissociative adsorption of vinyl bromide on Si(001): A first-principles study. *Physical Review B*, **2005**, 71,	3.3	10
63	Equivalence of electronic and mechanical stresses in structural phase stabilization: A case study of indium wires on Si(111). *Physical Review B*, **2015**, 91,	3.3	9
62	Self-assembly of molecular wires on H-terminated Si(100) surfaces driven by London dispersion forces. *Physical Review B*, **2011**, 84,	3.3	9
61	First-principles study of the adsorption and reaction of 2,3-butanediol on Si(001). *Physical Review B*, **2007**, 76,	3.3	9
60	Possibility of a ferromagnetic Rh(001) surface: A plane-wave-basis partial-core pseudopotential approach. *Physical Review B*, **1995**, 52, 13805-13807	3.3	9
59	Pseudopotential study of the structural properties of bulk Li. *Physical Review B*, **1993**, 47, 14020-14022	3.3	9
58	Stability and bonding nature of clathrate H cages in a near-room-temperature superconductor LaH10. *Physical Review Materials*, **2021**, 5,	3.2	9
57	Origin of Symmetric Dimer Images of Si(001) Observed by Low-Temperature Scanning Tunneling Microscopy. *Scientific Reports*, **2016**, 6, 27868	4.9	8
56	Peierls instability and ferrimagnetic ordering of quasi-one-dimensional carbon chains generated in H-passivated graphene. *Physical Review B*, **2011**, 83,	3.3	8
55	Peierls instability in one-dimensional borine wire on Si(001). *Journal of the American Chemical Society*, **2006**, 128, 11340-1	16.4	8
54	Abnormal volumetric thermal expansion in the hourglass fermion materials KHgAs and KHgSb. *Physical Review B*, **2017**, 95,	3.3	7
53	Quantum stability and magic lengths of metal atom wires. *Physical Review B*, **2016**, 93,	3.3	7
52	First-principles study of thermal and electron-activated dissociation of acetone on Si(001). *Journal of Chemical Physics*, **2008**, 129, 194110	3.9	7
51	Antiferromagnetic ordering in one-dimensional dangling-bond wires on a hydrogen-terminated C(001) surface: A density-functional study. *Physical Review B*, **2008**, 77,	3.3	7
50	Metastable phase of symmetric dimers on Si(001). *Physical Review B*, **2004**, 69,	3.3	7
49	Ab initio calculations of cyclopentene adsorbed on the diamond (001) surface. *Physical Review B*, **2002**, 65,	3.3	7

48	Comment on Identification of the Si 2p Surface Core Level Shifts on the Sb/Si(001)(2×1) Interface. *Physical Review Letters*, **1999**, 82, 4564-4564	7.4	7
47	Catalytic activities of noble metal atoms on WO3 (001): nitric oxide adsorption. *Nanoscale Research Letters*, **2015**, 10, 60	5	6
46	Nature of the Insulating Ground State of the Two-Dimensional Sn Atom Lattice on SiC(0001). *Scientific Reports*, **2016**, 6, 30598	4.9	6
45	Enhanced Stability and Electronic Structure of Phenylacetylene Lines on the Si(100)-(2×1):H Surface. *Journal of Physical Chemistry C*, **2011**, 115, 14942-14946	3.8	6
44	Self-directed growth of benzonitrile line on H-terminated Si(001) surface. *Journal of Chemical Physics*, **2004**, 121, 8010-3	3.9	6
43	Theoretical study of the structure of 1,5-cyclooctadiene on Si(001). *Physical Review B*, **2001**, 64,	3.3	6
42	Spontaneous Folding Growth of Graphene on h-BN. *Nano Letters*, **2021**, 21, 2033-2039	11.5	6
41	Two-dimensional topological semimetal states in monolayer Cu2Ge, Fe2Ge, and Fe2Sn. *Physical Review B*, **2020**, 101,	3.3	5
40	Comment on "Quasi-One-Dimensional Metal-Insulator Transitions in Compound Semiconductor Surfaces". *Physical Review Letters*, **2017**, 118, 239601	7.4	5
39	Competing charge density wave and antiferromagnetism of metallic atom wires in GaN(10$\bar{1}$0) and ZnO(10$\bar{1}$0). *Physical Review B*, **2017**, 96,	3.3	5
38	Giant spin-orbit-induced spin splitting in Bi zigzag chains on GaAs(110). *Physical Review B*, **2015**, 92,	3.3	5
37	Peierls Instability and Spin Orderings of Ultranarrow Graphene Nanoribbons in Graphane. *Journal of Physical Chemistry C*, **2012**, 116, 13795-13799	3.8	5
36	A density-functional-theory study of biradicals from benzene to hexacene. *Chemical Physics Letters*, **2011**, 516, 141-145	2.5	5
35	Theoretical prediction of the antiferromagnetic ground state of a C defect on Si(001). *Physical Review B*, **2009**, 80,	3.3	5
34	Zhang et al. Reply:. *Physical Review Letters*, **2011**, 107,	7.4	5
33	Density-Functional Calculations of the Adsorption and Reaction of Acetic Acid on Ge(001). *Journal of Physical Chemistry C*, **2008**, 112, 6947-6952	3.8	5
32	Si 2p core-level shifts at the C2H2/Si(001) and C2H4/Si(001) surfaces. *Physical Review B*, **2001**, 63,	3.3	5
31	Origin of enhanced chemical precompression in cerium hydride [Formula: see text]. *Scientific Reports*, **2020**, 10, 16878	4.9	5

30	Magnetic evolution and anomalous Wilson transition in diagonal phosphorene nanoribbons driven by strain. *Nanotechnology*, **2015**, 26, 295402	3.4	4
29	Self-directed growth approach for acetylacetone lines on an H-terminated Si(001)-(2 1) surface. *Physical Review B*, **2011**, 84,	3.3	4
28	Chiral Adsorption Structures of Styrene on Ge(001): A First-Principles Study. *Journal of Physical Chemistry C*, **2007**, 111, 5111-5114	3.8	4
27	Origin of surface metallization of Si(001) at high temperatures. *Physical Review B*, **2005**, 71,	3.3	4
26	Geometry and core-level shifts of As on GaAs(110). *Physical Review B*, **1999**, 59, 12200-12203	3.3	4
25	Dimensionality and Valency Dependent Quantum Growth of Metallic Nanostructures: A Unified Perspective. *Nano Letters*, **2016**, 16, 6628-6635	11.5	4
24	Evidence of Phonon-Mediated Superconductivity in LaH10 at High Pressure. *Annalen Der Physik*, **2021**, 533, 2000518	2.6	4
23	Contrasting diffusion behaviors of O and F atoms on graphene and within bilayer graphene. *Physical Chemistry Chemical Physics*, **2017**, 19, 9107-9112	3.6	3
22	Underlying mechanism of charge transfer in Li-doped MgH16 at high pressure. *Physical Review B*, **2020**, 102,	3.3	3
21	Atomic and electronic structure of doped Si(111)(23 3)R30?-Sn interfaces. *Physical Review B*, **2018**, 97,	3.3	3
20	Energetics and kinetics of Cu atoms and clusters on the Si(111)-7 7 surface: first-principles calculations. *Physical Chemistry Chemical Physics*, **2016**, 18, 18549-54	3.6	3
19	Competing edge structures of Sb and Bi bilayers generated by trivial and nontrivial band topologies. *Physical Review B*, **2018**, 98,	3.3	3
18	Antiferromagnetic spin ordering in the dissociative adsorption of H2 on Si(001): density-functional calculations. *Journal of Chemical Physics*, **2009**, 131, 244704	3.9	3
17	Antiferromagnetic ground state of a C(60)-covered Si(001) surface. *ChemPhysChem*, **2009**, 10, 334-6	3.2	3
16	Weak antiferromagnetic superexchange interaction in fcc C60Hn. *Physical Review B*, **2012**, 86,	3.3	3
15	Theoretical study of Na adsorption on top of In chains on the Si(111) surface. *Physical Review B*, **2002**, 66,	3.3	3
14	Quantum Size Effects in Metallic Overlayer Epitaxy. *Japanese Journal of Applied Physics*, **2000**, 39, 4302-4306	1.4	3
13	Pseudopotential study of the magnetic and metal-insulator transitions in metallic lithium. *Physical Review B*, **1994**, 49, 9555-9559	3.3	3

12	Origin of charge density wave in the layered kagome metal CsV3Sb5. *Physical Review B*, **2022**, 105,	3.3	3
11	Self-assembled line growth of allyl alcohol on the H-terminated Si(100)-(2×1) surface. *Surface Science*, **2012**, 606, 461-463	1.8	2
10	Length- and parity-dependent electronic states in one-dimensional carbon atomic chains on C(111). *Physical Review B*, **2010**, 82,	3.3	2
9	First-principles calculations of the structure and growth mechanism of allyl mercaptan lines on the H/Si(100)-2×1 surface. *Physical Review B*, **2011**, 83,	3.3	2
8	Hydrogen adsorption induced nanomagnetism at the Si(111)-(7×7) surface. *Physical Review B*, **2018**, 98,	3.3	2
7	Bulk structural properties of Mo: Plane-wave-basis pseudopotential study with a partial-core-correction scheme. *Physical Review B*, **1993**, 47, 2979-2982	3.3	1
6	Effect of hole doping on superconductivity in compressed CeH9 at high pressures. *Physical Review B*, **2021**, 104,	3.3	1
5	Formation Mechanism of Chemically Precompressed Hydrogen Clathrates in Metal Superhydrides. *Inorganic Chemistry*, **2021**, 60, 12934-12940	5.1	0
4	Antiferromagnetic ordering of dangling-bond electrons at the stepped Si(001) surface. *Journal of Chemical Physics*, **2013**, 138, 104702	3.9	
3	Structure and stability of one-dimensional o-phthalaldehyde lines on the Si(100)-2×1:H surface. *Physical Chemistry Chemical Physics*, **2011**, 13, 418-20	3.6	
2	Nanosession: Topological Effects109-114		
1	Phase transition of nanoscale Au atom chains on NiAl(110). *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2020**, 384, 126183	2.3	