

CITATION REPORT

List of articles citing

Ab initio molecular dynamics for liquid metals

DOI: 10.1103/physrevb.47.558
Physical Review B, 1993, 47, 558-561.

Source: <https://exaly.com/paper-pdf/24061009/citation-report.pdf>

Version: 2024-04-28

This report has been generated based on the citations recorded by exaly.com for the above article. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

#	Paper	IF	Citations
2243	Ab initio molecular dynamics for open-shell transition metals. <i>Physical Review B</i> , 1993 , 48, 13115-13118	3.3	5376
2242	ZnTe at high pressure: X-ray-absorption spectroscopy and x-ray-diffraction studies. <i>Physical Review B</i> , 1993 , 48, 8683-8693	3.3	64
2241	Structural and Electronic Properties of Clean and Hydrogenated Diamond (100) Surfaces. 1994 , 28, 659-664		61
2240	Theory of the crystal structures of selenium and tellurium: The effect of generalized-gradient corrections to the local-density approximation. <i>Physical Review B</i> , 1994 , 50, 13181-13185	3.3	229
2239	Ab initio molecular-dynamics study of structural, dynamical, and electronic properties of liquid Ge. <i>Physical Review B</i> , 1994 , 50, 8342-8347	3.3	46
2238	Packing Transitions in Nanosized Li Clusters. 1994 , 73, 3552-3555		60
2237	Ab initio molecular-dynamics simulation of the liquid-metal-amorphous-semiconductor transition in germanium. <i>Physical Review B</i> , 1994 , 49, 14251-14269	3.3	14561
2236	Ab initio calculation of the structural and electronic properties of carbon and boron nitride using ultrasoft pseudopotentials. <i>Physical Review B</i> , 1994 , 50, 15606-15622	3.3	326
2235	Norm-conserving and ultrasoft pseudopotentials for first-row and transition elements. 1994 , 6, 8245-8257		2570
2234	Cross-correlations between the Atomic and Electronic Structure and Dynamics of Liquid Metals. 1994 , 184, 45-63		
2233	Triplet structure of simple liquids. 1995 , 52, 2668-2675		4
2232	Atomic and electronic structure of icosahedral Al-Pd-Mn alloys and approximant phases. <i>Physical Review B</i> , 1995 , 51, 17355-17378	3.3	118
2231	Short-range order in crystalline, amorphous, liquid, and supercooled germanium probed by x-ray-absorption spectroscopy. <i>Physical Review B</i> , 1995 , 51, 12322-12336	3.3	134
2230	Vacancies and impurities in aluminum and magnesium. <i>Physical Review B</i> , 1995 , 52, 6313-6326	3.3	106
2229	Dynamical Properties of the Liquid Polyvalent Elements: Soft Modes in Liquids. 1995 , 29, 159-168		8
2228	Molecular modelling of the chemical interaction of atoms and molecules with a surface. 1995 , 64, 599-625		2
2227	Ab initio molecular dynamics for liquid metals. 1995 , 192-193, 222-229		502

2226	Ab initio Force Constant Approach to Phonon Dispersion Relations of Diamond and Graphite. 1995 , 32, 729-734		568
2225	The influence of generalized gradient corrections to the LDA on predictions of structural phase stability: the Peierls distortion in As and Sb. 1995 , 7, 3683-3692		28
2224	Dimer reconstruction and electronic surface states on clean and hydrogenated diamond (100) surfaces. <i>Physical Review B</i> , 1996 , 53, 7334-7351	3-3	222
2223	Structural and electronic properties of rhodium surfaces: an ab initio approach. 1996 , 346, 300-321		110
2222	Relaxation and electronic surface states of rhodium surfaces. 1996 , 352-354, 689-692		11
2221	(2 × 1) reconstruction and hydrogen-induced de-reconstruction of the diamond (100) and (111) surfaces. 1996 , 352-354, 745-749		44
2220	Surface reconstruction and electronic properties of clean and hydrogenated diamond (111) surfaces. 1996 , 357-358, 422-426		14
2219	Atomic and electronic structure of diamond (111) surfaces II. (2 × 1) and (√3 × √3) reconstructions of the clean and hydrogen-covered three dangling-bond surfaces. 1996 , 366, 464-482		34
2218	Atomic and electronic structure of diamond (111) surfaces I. Reconstruction and hydrogen-induced de-reconstruction of the one dangling-bond surface. 1996 , 366, 445-463		111
2217	Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. 1996 , 6, 15-50		41739
2216	Chemisorption of H on Pd(111): An ab initio approach with ultrasoft pseudopotentials. <i>Physical Review B</i> , 1996 , 54, 2157-2166	3-3	103
2215	Ab initio molecular dynamics applied to the dynamics of liquid metals and to the metal-non-metal transition. 1996 , 205-207, 833-840		32
2214	Quantum Steering Effects in the Dissociative Adsorption of H ₂ on Rh(100). 1996 , 77, 1119-1122		63
2213	Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. <i>Physical Review B</i> , 1996 , 54, 11169-11186	3-3	67107
2212	On conjugate gradient-like methods for eigen-like problems. 1996 , 36, 494-508		26
2211	LDA Predictions of C ₂₀ Isomerizations: Neutral and Charged Species. 1996 , 100, 6966-6972		62
2210	Ab initio calculations for SiC - Al interfaces: tests of electronic-minimization techniques. 1996 , 4, 397-408		44
2209	Structure and bonding of liquid Se. 1996 , 8, 9353-9357		17

2208	Ab initio calculations of the atomic and electronic structure of clean and hydrogenated diamond (110) surfaces. <i>Physical Review B</i> , 1997 , 56, 4203-4210	3-3	67
2207	Molecular Precursors in the Dissociative Adsorption of O ₂ on Pt(111). 1997 , 79, 4481-4484		293
2206	Role of silicon vacancies in yttrium-disilicide compounds from ab initio calculations. <i>Physical Review B</i> , 1997 , 55, 13479-13484	3-3	30
2205	Theoretical Investigation of Extended Defects in Group-III Nitrides. 1997 , 482, 808		2
2204	Polytypism and surface structure of SiC. 1997 , 6, 1346-1348		16
2203	H ₂ dissociative adsorption on Pd(111). <i>Physical Review B</i> , 1997 , 56, 15396-15403	3-3	143
2202	Ab initio simulation of the metal/nonmetal transition in expanded fluid mercury. <i>Physical Review B</i> , 1997 , 55, 7539-7548	3-3	106
2201	Ultrasoft pseudopotentials applied to magnetic Fe, Co, and Ni: From atoms to solids. <i>Physical Review B</i> , 1997 , 56, 15629-15646	3-3	302
2200	Atomic and electronic structure of diamond (111) surfaces: III. Electronic structure of the clean and hydrogen-covered three-dangling-bond surfaces. 1997 , 384, 94-105		12
2199	A systematic study of the surface energetics and structure of TiO ₂ (110) by first-principles calculations. 1997 , 385, 386-394		211
2198	A theoretical study of the H-induced reconstructions of the Pd(110) surface. 1997 , 377-379, 56-61		18
2197	Vibrational frequency and chemisorption site: a DFT-periodic study of NO on Pd (111) and Rh (111) surfaces. 1998 , 291, 15-23		129
2196	First-principles calculations of the radial breathing mode of single-wall carbon nanotubes. <i>Physical Review B</i> , 1998 , 58, R8869-R8872	3-3	274
2195	Model of the epitaxial growth of SiC-polytypes under surface-stabilized conditions. 1998 , 27, 848-852		25
2194	Ab initio molecular-dynamics studies of the graphitization of flat and stepped diamond (111) surfaces. <i>Physical Review B</i> , 1998 , 58, 13167-13175	3-3	50
2193	Ab-initio calculations of the 6D potential energy surfaces for the dissociative adsorption of H ₂ on the (100) surfaces of Rh, Pd and Ag. 1998 , 397, 116-136		83
2192	Structural and electronic properties of the MoS ₂ (101 0) edge-surface. 1998 , 407, 237-250		92
2191	The adsorption and dissociation of ROH molecules on TiO ₂ (110). 1998 , 409, 336-349		182

2190	Hydrogen adsorption on palladium: a comparative theoretical study of different surfaces. 1998 , 411, 123-136		172
2189	Ab initio study of the dissociative adsorption of H ₂ on the Pd(110) surface. 1998 , 412-413, 518-526		41
2188	First principles calculation of oxygen adsorption and reconstruction of Cu(110) surface. 1998 , 415, 194-211		79
2187	Adsorption of thiophene on RuS ₂ : An ab initio density-functional study. <i>Physical Review B</i> , 1998 , 58, R1782-R1785		36
2186	Phonon dispersion relation in rhodium: Ab initio calculations and neutron- scattering investigations. <i>Physical Review B</i> , 1998 , 57, 324-333	3-3	36
2185	First-order phase transitions by first-principles free-energy calculations: The melting of Al. <i>Physical Review B</i> , 1998 , 57, 8223-8234	3-3	115
2184	Adsorption of Methanol on TiO ₂ (110): A First-Principles Investigation. 1998 , 102, 2017-2026		114
2183	Local order in liquid potassium-antimony alloys studied by neutron scattering and ab initio molecular dynamics. 1998 , 43, 539-545		10
2182	Acetylene structure and dynamics on Pd(111). <i>Physical Review B</i> , 1998 , 57, R12705-R12708	3-3	60
2181	Ab initio calculations of the atomic and electronic structure of diamond (111) surfaces with steps. <i>Physical Review B</i> , 1998 , 58, 2161-2169	3-3	21
2180	Structure and dynamics of liquid selenium. <i>Physical Review B</i> , 1998 , 57, 10482-10495	3-3	76
2179	Si-rich SiC(111)/(0001)3B and 3B surfaces: A Mott-Hubbard picture. <i>Physical Review B</i> , 1998 , 58, 13712-13716	3-3	71
2178	Ab initio calculations of the structural properties of the YSi ₂ (0001) surface. <i>Physical Review B</i> , 1998 , 58, 10857-10859	3-3	11
2177	Interlayer Self-Diffusion on Stepped Pt(111). 1998 , 81, 168-171		110
2176	Reversed spin polarization at the Co(001)-HfO ₂ (001) interface. <i>Physical Review B</i> , 1998 , 58, 15422-15425	3-3	13
2175	Ab initio studies of the (111) and (111) surfaces of cubic BN: Structure and energetics. <i>Physical Review B</i> , 1998 , 58, 15636-15646	3-3	23
2174	Adsorption of CO on Rh(100) studied by ab initio local-density functional calculations. 1998 , 109, 5585-5595		44
2173	Bond-rotation versus bond-contraction relaxation of (110) surfaces of group-III nitrides. <i>Physical Review B</i> , 1998 , 58, R1722-R1725	3-3	64

2172	H-induced reconstructions on Pd(110). <i>Physical Review B</i> , 1998 , 57, 12482-12491	3-3	40
2171	Adsorption of CO on Pd(100): Steering into less favored adsorption sites. <i>Physical Review B</i> , 1998 , 57, 10110-10114	3-3	40
2170	Novel Reconstruction Mechanism for Dangling-Bond Minimization: Combined Method Surface Structure Determination of SiC(111)- (3 $\bar{2}$). 1998 , 80, 758-761		162
2169	High Pressure Polymorphism in Silica. 1998 , 80, 2145-2148		190
2168	Vibrations of O on stepped Pt(111). <i>Physical Review B</i> , 1998 , 58, 2179-2184	3-3	29
2167	Carbon vacancy in SiC: A negative- U system. 1998 , 44, 309-314		17
2166	FirstPrinciples Investigation of the Ordered Si 4c compound. 1998 , 535, 299		1
2165	Exploring the Excited States of Vacancy Defects in Silica. 1998 , 540, 379		2
2164	Theoretical study of benzothiophene hydrodesulfurization on MoS ₂ . 1999 , 127, 327-334		22
2163	STRUCTURE AND DYNAMICS OF Al TRIMER ON Al(111) SURFACE. 1999 , 06, 787-792		
2162	Electronic structure of the (111) and (1 $\bar{1}$ 1 $\bar{1}$) surfaces of cubic BN: A local-density-functional ab initio study. <i>Physical Review B</i> , 1999 , 60, 8719-8726	3-3	7
2161	Reaction channels for the catalytic oxidation of CO on Pt(111). <i>Physical Review B</i> , 1999 , 59, 5960-5967	3-3	92
2160	Variations in the Nature of Metal Adsorption on Ultrathin Al ₂ O ₃ Films. 1999 , 82, 4050-4053		160
2159	Anomalous behavior of the semiconducting gap in WO ₃ from first-principles calculations. <i>Physical Review B</i> , 1999 , 59, 2684-2693	3-3	109
2158	First-principles step- and kink-formation energies on Cu(111). <i>Physical Review B</i> , 1999 , 60, 11118-11122	3-3	34
2157	A Full-Potential LMTO Method Based on Smooth Hankel Functions. 1999 , 114-147		97
2156	Dissociation of water on the surface of galena (PbS): A comparison of periodic and cluster models. 1999 , 111, 6942-6946		23
2155	Adsorption-induced lattice relaxation and diffusion by concerted substitution. <i>Physical Review B</i> , 1999 , 59, 5892-5897	3-3	33

2154	29Si NMR study on the stoichiometry of the silicon clathrate Na ₈ Si ₄₆ . <i>Physical Review B</i> , 1999 , 60, 12294-12298	3-3	11
2153	Interpretation of O binding-site preferences on close-packed group-VIII metal surfaces. <i>Physical Review B</i> , 1999 , 59, 2327-2331	3-3	11
2152	Band-gap and k.p. parameters for GaAlN and GaInN alloys. 1999 , 86, 3768-3772		36
2151	Atomic structure of the c(2×2) Si/Cu(110) surface alloy from ab initio calculation. <i>Physical Review B</i> , 1999 , 60, 6034-6038	3-3	6
2150	Polyanionic and octet phases in the K-Sb system. I. Crystalline intermetallic compounds. <i>Physical Review B</i> , 1999 , 59, 829-842	3-3	16
2149	Influence of crystal structure on the lattice sites and formation energies of hydrogen in wurtzite and zinc-blende GaN. <i>Physical Review B</i> , 1999 , 60, R5101-R5104	3-3	39
2148	Large Fermi Density Waves on the Reconstructed Pt(100) Surface. 1999 , 83, 2604-2607		10
2147	Dislocation Structures of Submonolayer Films near the Commensurate-Incommensurate Phase Transition: Ag on Pt(111). 1999 , 82, 4488-4491		25
2146	Ab Initio Molecular Dynamics Studies of Off-Center Displacements in CuCl. 1999 , 83, 568-571		14
2145	Simulations of fluid hydrogen: comparison of a dissociation model with tight-binding molecular dynamics. 1999 , 60, 1665-73		17
2144	Metal-on-Metal Bonding and Rebonding Revisited. 1999 , 82, 5301-5304		24
2143	Density functional periodic study of CO adsorption on the Pd ₃ Mn(100) alloy surface: Comparison with Pd(100). <i>Physical Review B</i> , 1999 , 59, 5142-5153	3-3	44
2142	Electronic structure study of liquid germanium based on x-ray-absorption near-edge structure spectroscopy. <i>Physical Review B</i> , 1999 , 59, 1571-1574	3-3	6
2141	Ab initio study of phonons in hexagonal GaN. <i>Physical Review B</i> , 1999 , 60, 15511-15514	3-3	37
2140	Modeling STM tips by single absorbed atoms on W(100) films: 5d transition metal atoms. 1999 , 113, 245-250		19
2139	An order(N) tight-binding molecular dynamics study of intrinsic defect diffusion in silicon. 1999 , 74, 67-75		8
2138	First-principles molecular dynamics study of small molecules in zeolites. 1999 , 50, 501-509		27
2137	Monovacancies in 3C and 4H SiC. 1999 , 61-62, 244-247		7

2136	Transition metals to sulfur binding energies relationship to catalytic activities in HDS: back to Sabatier with first principle calculations ¹ This work has been undertaken within the IDR Dynamique Moléculaire Quantique Appliquée à la Catalyse, a joint project of Centre National de la Recherche Scientifique, Technische Universität Wien, and Institut Français du Pétrole.1. 1999 , 50, 629-636		128
2135	Soft X-ray fluorescence spectra of photoluminescent layered polysilanes. 1999 , 301, 474-480		1
2134	Pairing in dense lithium. 1999 , 400, 141-144		328
2133	Catalysis of the reaction HCl+HOCl-H ₂ O+Cl ₂ on an ice surface. 1999 , 309, 335-343		22
2132	Ab initio molecular dynamics study on the hydrolysis of molecular chlorine. 1999 , 311, 93-101		12
2131	Ab initio molecular dynamics study on the thermal dissociation of acetic acid. 1999 , 314, 317-325		17
2130	Vacancies in SiC: Influence of Jahn-Teller distortions, spin effects, and crystal structure. <i>Physical Review B</i> , 1999 , 59, 15166-15180	3-3	211
2129	Determination of Band Structure Parameters in Nitride Alloys for Use in Quantum Well Calculations. 1999 , 216, 351-354		
2128	Ab initio calculation of the lattice dynamics and phase diagram of boron nitride. <i>Physical Review B</i> , 1999 , 59, 8551-8559	3-3	303
2127	Structure and electronic properties of amorphous WO ₃ . <i>Physical Review B</i> , 1999 , 60, 16463-16474	3-3	79
2126	Why Pb(B,B')O ₃ perovskites disorder at lower temperatures than Ba(B,B')O ₃ perovskites. <i>Physical Review B</i> , 1999 , 60, R12542-R12545	3-3	78
2125	Mechanism of Boron Diffusion in Silicon: An Ab Initio and Kinetic Monte Carlo Study. 1999 , 83, 4341-4344		161
2124	Theoretical study of two expanded phases of crystalline germanium: clathrate-I and clathrate-II. 1999 , 11, 6129-6145		66
2123	Theoretical study of the vibrational modes and their pressure dependence in the pure clathrate-II silicon framework. <i>Physical Review B</i> , 1999 , 60, 950-958	3-3	84
2122	First-principles calculations to describe zirconia pseudopolymorphs. <i>Physical Review B</i> , 1999 , 59, 4044-4053	3-3	151
2121	Retardation of O diffusion through polycrystalline Pt by Be doping. <i>Physical Review B</i> , 1999 , 59, 16047-16052	3-3	11
2120	First-Principles Study of Boron Diffusion in Silicon. 1999 , 83, 4345-4348		188
2119	Why clathrates are good thermoelectrics: A theoretical study of Sr ₈ Ga ₁₆ Ge ₃₀ . 1999 , 111, 3133-3144		116

2118	The electronic structure and transport properties of clathrates: a density functional study.		
2117	Geometry and electronic structure of magic iron oxide clusters. <i>Physical Review B</i> , 1999 , 59, 12672-12677	3,3	46
2116	Structural, electronic and magnetic properties of nickel surfaces. 1999 , 423, 1-11		106
2115	Reaction channels for the catalytic oxidation of CO on Pt(111). 1999 , 433-435, 58-62		45
2114	Dependence of stretching frequency on surface coverage and adsorbate-adsorbate interactions: a density-functional theory approach of CO on Pd (111). 1999 , 425, 68-80		165
2113	Molecular precursors in the dissociative adsorption of O ₂ on Ni(111). 1999 , 433-435, 756-760		39
2112	SiCl ₄ desorption in chlorine etching of Si(100) - a first principles study. 1999 , 432, 125-138		4
2111	Density functional study of the structural and electronic properties of RuS ₂ (111): I. Bare surfaces. 1999 , 439, 163-172		13
2110	NO chemisorption on a magnetic alloy surface: a density-functional periodic study of Pd ₃ Mn(100) compared with Pd(100). 1999 , 442, 338-348		24
2109	Structure of liquid potassium-antimony alloys: neutron scattering experiments and ab initio molecular dynamics calculations. 1999 , 250-252, 253-257		6
2108	Band structure of In _x Ga _{1-x} As _{1-y} N _y alloys and effects of pressure. <i>Physical Review B</i> , 1999 , 60, 4430-4433	3,3	166
2107	Polycarbon Ligand Chemistry: Electronic Interactions between a Mononuclear Ruthenium Fragment and a Cobalt-Carbon Cluster Core. 1999 , 18, 3885-3897		46
2106	Electronic structure calculations on nitride semiconductors. 1999 , 14, 23-31		142
2105	Role of surface vacancies and water products in metal nucleation: Pt/MgO(100). 1999 , 437, L741-L747		92
2104	Self-diffusion along step bottoms on Pt(111). <i>Physical Review B</i> , 1999 , 60, 4972-4981	3,3	41
2103	High-pressure x-ray absorption study of InSe. <i>Physical Review B</i> , 1999 , 60, 3757-3763	3,3	26
2102	Ab-initio energy profiles for thiophene HDS on the MoS ₂ (1010) edge-surface. 1999 , 127, 309-317		18
2101	Ab-Initio Pseudopotential Calculations of Boron Diffusion in Silicon. 1999 , 568, 91		5

2100	Microscopic and Theoretical Investigations of the Si-SiO ₂ Interface. 1999 , 592, 42	1
2099	Atomic Structure of Pd-Intercalated Graphite by High-Resolution Electron Microscopy and First Principles Calculations. 1999 , 40, 1213-1218	3
2098	Effect of Lattice Coherency on Solution Energies of Impurities: Stability of an Epitaxial InAs Monolayer Deposited on GaAs. 1999 , 40, 1295-1300	
2097	Ab-Initio Studies of AlSb (001) Adatom Behavior and Reconstruction. 2000 , 618, 11	
2096	Fundamental Cluster and Hydrogen Sites in Ti-Zr-Ni Quasicrystals. 2000 , 643, 521	
2095	Grain boundary structure in B2 Fe-Al ordered alloys: an atomic-scale simulation. 2000 , 652, 1	
2094	Atomic Scale Simulation of the Effect of Hydrogen on Dislocations in Zr. 2000 , 653, 1	
2093	Hydrogen and hot electron defect creation at the Si(100)/SiO ₂ interface of metal-oxide-semiconductor field effect transistors. 2000 , 27, 229-233	10
2092	Dissociative chemisorption of molecular chlorine on Si(100) by first principles study. 2000 , 318, 15-21	3
2091	The adsorption of aromatics on sp-metals: benzene on Al(111). 2000 , 318, 43-48	62
2090	Defect study on Ce ³⁺ in LiBaF ₃ . 2000 , 87-89, 1023-1025	6
2089	The Raman spectra of the hexagonal and cubic (spinel) forms of Ge ₃ N ₄ : an experimental and theoretical study. 2000 , 114, 137-142	30
2088	Structural modelling of the TiZrNi quasicrystal. 2000 , 294-296, 361-365	27
2087	An ab initio based structure model of i(AlPdMn). 2000 , 294-296, 351-354	0
2086	Development of glue-type potentials for the AlPd system: phase diagram calculation. 2000 , 48, 1753-1761	65
2085	Co-deposition of In and Sn on the Si(100) 2x1 surface: growth of a one-dimensional alloy?. 2000 , 162-163, 638-643	7
2084	Six-dimensional classical dynamics of H ₂ dissociative adsorption on Pd(111). 2000 , 320, 328-334	54
2083	Why Pb(B ₁ /3B ₂ /3)O ₃ perovskites disorder more easily than Ba(B ₁ /3B ₂ /3)O ₃ perovskites and the thermodynamics of 1:1-type short-range order in PMN. 2000 , 61, 327-333	27

2082	Self-trapped excitons in quartz. 2000 , 166-167, 451-458			17
2081	Quantum study of the active sites of the alumina surface: chemisorption and adsorption of water, hydrogen sulfide and carbon monoxide on aluminum and oxygen sites. 2000 , 505, 81-94			43
2080	Ab Initio Study of the H ₂ /2S/MoS ₂ Gas/Solid Interface: The Nature of the Catalytically Active Sites. 2000 , 189, 129-146			292
2079	Structure, Energetics, and Electronic Properties of the Surface of a Promoted MoS ₂ Catalyst: An ab Initio Local Density Functional Study. 2000 , 190, 128-143			266
2078	Phase stability and structure of spinel-based transition aluminas. <i>Physical Review B</i> , 2000 , 63,	3-3		198
2077	Boron diffusion and activation in the presence of other species.			1
2076	Dielectric and lattice-dynamical properties of III-nitrides. 2000 , 29, 281-284			4
2075	Interface assisted formation of a metastable hcp phase by ion mixing in an immiscible Ag-Ni system. 2000 , 12, 9231-9235			5
2074	Strain-induced tetragonal distortions in epitaxial Ni-films grown on Cu(001). 2000 , 12, L139-L146			16
2073	²³ Na and ²⁹ Si NMR Knight shifts in the silicon clathrate Na ₁₆ Cs ₈ Si ₁₃₆ . <i>Physical Review B</i> , 2000 , 63,	3-3		17
2072	C incorporation mechanisms on Si(001) investigated by ab initio calculations. <i>Physical Review B</i> , 2000 , 62, 5021-5027	3-3		10
2071	Ordering of self-diffusion barrier energies on Pt(110)-(1 \times 1). <i>Physical Review B</i> , 2000 , 61, R2452-R2455	3-3		26
2070	Pairing, Bonding, and the role of nonlocality in a dense lithium monolayer. <i>Physical Review B</i> , 2000 , 62, 8494-8499	3-3		32
2069	Density-functional calculation of the Hugoniot of shocked liquid deuterium. <i>Physical Review B</i> , 2000 , 61, 1-4	3-3		159
2068	C incorporation in epitaxial Ge _{1-x} Cy layers grown on Ge(001): An ab initio study. <i>Physical Review B</i> , 2000 , 62, R7723-R7726	3-3		19
2067	Atom-by-atom and concerted hopping of adatom pairs on an open metal surface. <i>Physical Review B</i> , 2000 , 61, R2456-R2459	3-3		12
2066	Stability of Si-interstitial defects: from point to extended defects. 2000 , 84, 503-6			130
2065	Possible metastable states in the Ni-W system predicted by ab initio calculations. <i>Physical Review B</i> , 2000 , 62, 11277-11279	3-3		10

2064	Energetics and diffusion of hydrogen in SiO ₂ . <i>Physical Review B</i> , 2000 , 61, 4417-4420	3-3	51
2063	Density-functional calculation of the Hugoniot of shocked liquid nitrogen. <i>Physical Review B</i> , 2000 , 63,	3-3	43
2062	Excitonic effects in core-excitation spectra of semiconductors. 2000 , 85, 2168-71		69
2061	Structure and magnetism of Fe overlayers on face-centered-cubic Co(001) substrates. <i>Physical Review B</i> , 2000 , 62, 9575-9585	3-3	14
2060	Self-diffusion of small clusters on fcc metal (111) surfaces. 2000 , 85, 1044-7		63
2059	Lithium trapping by excess oxygen in WO ₃ : A first-principles study. <i>Physical Review B</i> , 2000 , 62, 1508-1513	3-3	6
2058	Theoretical study of Fe ₃ N ₄ and its high-pressure spinel phase. <i>Physical Review B</i> , 2000 , 61, 11979-11992	3-3	79
2057	Calculating properties with the polymorphous coherent-potential approximation. <i>Physical Review B</i> , 2000 , 61, 12005-12016	3-3	28
2056	Structures of magic Ba clusters and magic Ba suboxide clusters. 2000 , 62,		15
2055	Structure, optical absorption, and luminescence energy calculations of Ce ³⁺ defects in LiBaF ₃ . <i>Physical Review B</i> , 2000 , 61, 16477-16490	3-3	46
2054	Photoluminescence-linewidth-derived reduced exciton mass for In _y Ga _{1-y} As _{1-x} N _x alloys. <i>Physical Review B</i> , 2000 , 62, 7144-7149	3-3	26
2053	First-principles studies on the intrinsic stability of the magic Fe ₁₃ O ₈ cluster. <i>Physical Review B</i> , 2000 , 61, 5781-5785	3-3	21
2052	Structure of III-Sb(001) growth surfaces: the role of heterodimers. 2000 , 84, 4649-52		66
2051	Formation and diffusion of S-decorated Cu clusters on Cu(111). 2000 , 85, 606-9		81
2050	Nature, strength, and consequences of indirect adsorbate interactions on metals. 2000 , 85, 1910-3		167
2049	Local-spin-density-approximation molecular-dynamics simulations of dense deuterium. 2001 , 63, 015301		36
2048	Ab initio energetics of boron-interstitial clusters in crystalline Si. 2000 , 77, 1834		57
2047	Toward control of surface reactions with a scanning tunneling microscope. Structure and dynamics of benzene desorption from a silicon surface. 2000 , 113, 4412-4423		41

2046	Band offsets and stability of BeTe/ZnSe (100) heterojunctions. <i>Physical Review B</i> , 2000 , 62, R16302-R16305	3-3	14
2045	Investigation of hardness in tetrahedrally bonded nonmolecular CO ₂ solids by density-functional theory. <i>Physical Review B</i> , 2000 , 62, 14685-14689	3-3	54
2044	First-principles characterization of a heteroceramic interface: ZrO ₂ (001) deposited on an Al ₂ O ₃ (110 ₂) substrate. <i>Physical Review B</i> , 2000 , 62, 16968-16983	3-3	56
2043	NMR second-moment study of hydrogen sites in icosahedral Ti ₄₅ Zr ₃₈ Ni ₁₇ quasicrystals. <i>Physical Review B</i> , 2000 , 62, 11444-11449	3-3	14
2042	Rigid intertetrahedron angular interaction of nonmolecular carbon dioxide solids. <i>Physical Review B</i> , 2000 , 61, 5967-5971	3-3	47
2041	Ab initio step and kink formation energies on Pb(111). <i>Physical Review B</i> , 2000 , 62, 17020-17025	3-3	32
2040	Structural, electronic, and magnetic properties of thin Mn/Cu(100) films. <i>Physical Review B</i> , 2000 , 61, 11492-11505	3-3	63
2039	Geometry and electronic structures of magic transition-metal oxide clusters M ₉ O ₆ (M=Fe, Co, and Ni). <i>Physical Review B</i> , 2000 , 62, 8500-8507	3-3	39
2038	Adsorption energetics and bonding from femtomole calorimetry and from first principles theory. 2000 , 45, 207-259		37
2037	Highly optimized empirical potential model of silicon. 2000 , 8, 825-841		127
2036	Kinetic Monte Carlo simulations of cascades in Fe alloys. 2000 , 650, 3251		7
2035	Dissociation pathways of oxygen on copper (110) surface: a first principles study. 2000 , 17, 133-140		21
2034	In, Sn dimers on Si(100)2x1 surface: ab initio calculations and STM experiments. 2000 , 454-456, 489-493		17
2033	Adsorption of group III atoms on SiC(111) surfaces. 2000 , 454-456, 127-130		1
2032	Adsorption and energetics of isolated CO molecules on Pd(111). 2000 , 453, 25-31		64
2031	Atomic and electronic structure of the (111) surface of cubic BN: an LDF ab initio study. 2000 , 454-456, 494-497		8
2030	Density functional theory calculations of adsorption of water at calcium oxide and calcium fluoride surfaces. 2000 , 452, 9-19		75
2029	Density functional study of the structural and electronic properties of RuS ₂ (111): II. Hydrogenated surfaces. 2000 , 457, 285-293		13

2028	Pathways to dissociation of O ₂ on Cu (110) surface: first principles simulations. 2000 , 459, 104-114		42
2027	Ultrathin aluminum oxide films: Al-sublattice structure and the effect of substrate on ad-metal adhesion. 2000 , 464, 108-116		53
2026	Energetics and structure of stoichiometric SnO ₂ surfaces studied by first-principles calculations. 2000 , 463, 93-101		236
2025	Step- versus kink-formation energies on Pt(111). 2000 , 463, L661-L665		19
2024	Surface and subsurface alloy formation of vanadium on Pd(111). 2000 , 463, 199-210		42
2023	Structural and dynamical behavior of Al trimer on Al(111) surface. 2000 , 465, 65-75		15
2022	Cu interactions with β -Al ₂ O ₃ (0001): effects of surface hydroxyl groups versus dehydroxylation by Ar-ion sputtering. 2000 , 465, 163-176		90
2021	The energetics and structure of oxygen vacancies on the SnO ₂ (110) surface. 2000 , 467, 35-48		74
2020	Limits of perturbation theory: first principles simulations of scanning tunneling microscopy scans on Fe(100). 2000 , 466, L795-L801		28
2019	Copper wetting of β -Al ₂ O ₃ (0001): theory and experiment. 2000 , 446, 76-88		88
2018	Electron-stimulated bond rearrangements on the H/Si(100)-3 \times 1 surface. 2000 , 446, 211-218		16
2017	Phonons and static dielectric constant in CaTiO ₃ from first principles. <i>Physical Review B</i> , 2000 , 62, 3735-3743		155
2016	Dynamics and polarization of group-III nitride lattices: A first-principles study. <i>Physical Review B</i> , 2000 , 62, 8003-8011	3-3	98
2015	Long-range versus short-range interactions and the configurational energies of Ba(B,B')O ₃ and Pb(B,B')O ₃ perovskites. 2000 , 8, 211-219		6
2014	Compact surface-cluster diffusion by concerted rotation and translation. <i>Physical Review B</i> , 2000 , 61, R5125-R5128	3-3	24
2013	Comment on Assignment of the Raman active vibration modes of β -Si ₃ N ₄ using micro-Raman scattering [J. Appl. Phys. 85, 7380 (1999)]. 2000 , 87, 958-959		19
2012	Theoretical Study of the MoS ₂ (100) Surface: A Chemical Potential Analysis of Sulfur and Hydrogen Coverage. 2000 , 104, 11220-11229		143
2011	Ab initio calculations of phonons in LiNbO ₃ . <i>Physical Review B</i> , 2000 , 61, 272-278	3-3	89

2010	Diffusion of Ge below the Si(100) surface: theory and experiment. 2000 , 84, 2441-4		70
2009	Ab initio investigation of C incorporation mechanisms on Si(001). 2000 , 76, 885-887		23
2008	Energetics of hydrogen chemisorbed on Cu(110): A first principles calculations study. 2000 , 113, 6926-6932		31
2007	First-Principles Studies on Pd Intercalated Graphite. 2000 , 340, 283-288		1
2006	Bond Scission in a Perfect Polyethylene Chain and the Consequences for the Ultimate Strength. 2000 , 33, 9098-9108		25
2005	Precursor-mediated adsorption of oxygen on the (111) surfaces of platinum-group metals. <i>Physical Review B</i> , 2000 , 62, 4744-4755	3-3	302
2004	O/N Ordering in Y ₂ Si ₃ O ₃ N ₄ with the Melilite-type Structure from First-Principles Calculations. 2000 , 12, 1071-1075		27
2003	Synthesis and crystal structure determination of a new pressure-induced iridium ditelluride phase, m-IrTe ₂ , and comparison of the crystal structures and relative stabilities of various IrTe ₂ polymorphs. 2000 , 39, 4370-3		9
2002	Direct calculation of k _p parameters for wurtzite AlN, GaN, and InN. <i>Physical Review B</i> , 2000 , 61, 12933-12938	3-3	60
2001	Oxametallacycle Intermediates on Clean and Cs-Promoted Ag(111) Surfaces. 2000 , 104, 8685-8691		27
2000	High-pressure x-ray absorption study of GaTe including polarization. <i>Physical Review B</i> , 2000 , 61, 125-131	3-3	12
1999	Integrated Experimental and Computational Methods for Structure Determination and Characterization of a New, Highly Stable Cesium Silicotitanate Phase, Cs ₂ TiSi ₆ O ₁₅ (SNL-A). 2000 , 12, 3449-3458		34
1998	The Hydration Number of Li ⁺ in Liquid Water. 2000 , 122, 966-967		192
1997	Bulk and Surface Electronic Structure of the Layered Sub-Nitrides Ca ₂ N and Sr ₂ N. 2000 , 12, 1847-1852		22
1996	High pressure-high temperature synthesis and elasticity of the cubic nitride spinel Si ₃ N ₄ . 2001 , 13, 557-563		76
1995	Structural and electronic properties of tin clathrate materials. <i>Physical Review B</i> , 2001 , 64,	3-3	59
1994	Nonlinear macroscopic polarization in III-V nitride alloys. <i>Physical Review B</i> , 2001 , 64,	3-3	238
1993	Search for ultra-hard materials: theoretical characterisation of novel orthorhombic BC ₂ N crystals. 2001 , 3, 943-957		61

1992	Structural stability and lattice defects in copper: Ab initio, tight-binding, and embedded-atom calculations. <i>Physical Review B</i> , 2001 , 63,	3-3	1500
1991	Metallic Character of the Al ₂ O ₃ (0001)-(√3 × √3)R ⁻ 9° Surface Reconstruction. 2001 , 105, 4045-4052		52
1990	Initial adsorption configurations of acetylene molecules on the Si(001) surface. <i>Physical Review B</i> , 2001 , 64,	3-3	62
1989	Density Functional Theory Calculations of Hydrogen-Containing Defects in Forsterite, Periclase, and β -Quartz. 2001 , 105, 9747-9754		50
1988	Atomic-scale characterization of boron diffusion in silicon. <i>Physical Review B</i> , 2001 , 64,	3-3	40
1987	Defect-induced nonpolar-to-polar transition at the surface of chalcopyrite semiconductors. <i>Physical Review B</i> , 2001 , 64,	3-3	101
1986	Phase stabilities and structural relaxations in substoichiometric TiC _{1-x} . <i>Physical Review B</i> , 2001 , 63,	3-3	117
1985	Concerted Use of Slab and Cluster Models in an ab Initio Study of Hydrogen Desorption from the Si(100) Surface 2001 , 105, 4031-4038		39
1984	Second nearest-neighbor modified embedded atom method potentials for bcc transition metals. <i>Physical Review B</i> , 2001 , 64,	3-3	422
1983	Modeling STM tips by single adsorbed atoms on W(100) films: 3d and 4d transition-metal atoms. <i>Physical Review B</i> , 2001 , 64,	3-3	15
1982	Ab initio study of the vibrational and electronic properties of CdGa ₂ S ₄ and CdGa ₂ Se ₄ under pressure. 2001 , 13, 10117-10124		17
1981	Proof of the thermodynamical stability of the E' center in SiO ₂ . 2001 , 86, 3064-7		45
1980	Ab initio calculations of defects in Fe and dilute Fe-Cu alloys. <i>Physical Review B</i> , 2001 , 65,	3-3	346
1979	Defect ordering in aliovalently doped cubic zirconia from first principles. <i>Physical Review B</i> , 2001 , 64,	3-3	141
1978	Ab initio molecular-dynamics study of highly nonideal structural and thermodynamic properties of liquid Ni-Al alloys. <i>Physical Review B</i> , 2001 , 64,	3-3	22
1977	First-principles studies on pure and doped C ₃₂ clusters. 2001 , 13, 1931-1938		12
1976	Hydrogen Adsorption in Potassium-Intercalated Graphite of Second Stage: An ab Initio Molecular Dynamics Study. 2001 , 105, 736-742		20
1975	Optical properties of semiconductors using projector-augmented waves. <i>Physical Review B</i> , 2001 , 63,	3-3	238

1974	Theoretical study of alkali-atom insertion into small-radius carbon nanotubes to form single-atom chains. <i>Physical Review B</i> , 2001 , 64,	3-3	45
1973	Long time scale kinetic Monte Carlo simulations without lattice approximation and predefined event table. 2001 , 115, 9657-9666		358
1972	Spin-dependent tunneling conductance of Fe MgO Fe sandwiches. <i>Physical Review B</i> , 2001 , 63,	3-3	1598
1971	Theoretical structure determination of α -Al ₂ O ₃ . <i>Physical Review B</i> , 2001 , 65,	3-3	181
1970	Theoretical Study of the Dehydration Process of Boehmite to γ -Alumina. 2001 , 105, 5121-5130		362
1969	Molecular Dynamics Simulations of Pd Deposition on the α -Al ₂ O ₃ (0001) Surface. 2001 , 105, 12111-12117		24
1968	Lattice dynamics of cubic BN. 2001 , 328, 97-99		27
1967	First-principles characterisation of new ternary heterodiamond BC ₂ N phases. 2001 , 20, 107-119		64
1966	Energetics and diffusivity of atomic boron in silicon by density-functional-based tight-binding simulations. 2001 , 22, 44-48		10
1965	Ab initio modeling study of boron diffusion in silicon. 2001 , 21, 496-504		9
1964	Structure and reactivity of amorphous silicon nitride investigated with density-functional methods. 2001 , 293-295, 238-243		30
1963	Atomic networks and clustering in liquid Te and KTe alloys. 2001 , 293-295, 193-198		15
1962	Cu, Ag, and Au atoms adsorbed on TiO ₂ (110): cluster and periodic calculations. 2001 , 471, 21-31		117
1961	Density-functional study of the adsorption of benzene on the (111), (100) and (110) surfaces of nickel. 2001 , 472, 133-153		114
1960	STM-induced void formation at the Al ₂ O ₃ /Ni ₃ Al(1 1 1) interface. 2001 , 472, L157-L163		12
1959	Adsorption sites and STM images of C ₂ H ₂ on Si(100): a first-principles study. 2001 , 475, 83-88		36
1958	Quenching surface states with the tip: STM scans on Fe(1 0 0). 2001 , 482-485, 1113-1118		8
1957	Stability, electronic properties and chemical reactivity of palladium-manganese(1 1 1) surface alloys. 2001 , 482-485, 712-717		12

1956	Accelerated mound decay at adjacent kinks on Cu(111). 2001 , 478, L349-L354	11
1955	Weak bonding of alumina coatings on Ni(111). 2001 , 487, 55-76	45
1954	The first-principle study of the iodine-modified silver surfaces. 2001 , 487, 77-86	21
1953	Physisorption of water on salt surfaces. 2001 , 488, 177-192	37
1952	Structural and electronic properties of silver surfaces: ab initio pseudopotential density functional study. 2001 , 490, 125-132	41
1951	First-principles study of the interaction of oxygen with the SnO ₂ (110) surface. 2001 , 490, 221-236	82
1950	A theoretical investigation of the binding of TiCl _n to MgCl ₂ . 2001 , 490, 237-250	35
1949	A DFT study of the adsorption of thiophene on Ni(100). 2001 , 492, 27-33	32
1948	Pt-dimer dissociation on Pt(111). 2001 , 492, L723-L728	15
1947	Structure of an ultrathin TiO _x film, formed by the strong metal support interaction (SMSI), on Pt nanocrystals on TiO ₂ (110). 2001 , 492, L677-L687	70
1946	Application of ab initio molecular dynamics for a priori elucidation of the mechanism in unimolecular decomposition: the case of 5-nitro-2,4-dihydro-3H-1,2,4-triazol-3-one (NTO). 2001 , 123, 2243-50	44
1945	Breaking the NO bond on Rh, Pd, and Pd ₃ Mn alloy (100) surfaces: A quantum chemical comparison of reaction paths. 2001 , 115, 8101-8111	51
1944	CO Adsorption on Pt ₃ Bu Surface Alloys and on the Surface of Pt ₃ Bu Bulk Alloy. 2001 , 105, 9533-9536	77
1943	Alloying Effects on N ₂ Stretching Frequency: A Density Functional Theory Study of the Adsorption of NO on Pd ₃ Mn (100) and (111) Surfaces. 2001 , 105, 3027-3033	12
1942	Structure and Energetics of Iron Pentacarbonyl Formation at an Fe(100) Surface. 2001 , 105, 12547-12552	33
1941	Density of constitutional and thermal point defects in L12 Al ₃ Sc. <i>Physical Review B</i> , 2001 , 63, 3-3	54
1940	Ab initio study of deuterium in the dissociating regime: sound speed and transport properties. 2001 , 64, 066406	27
1939	Dynamical and optical properties of warm dense hydrogen. <i>Physical Review B</i> , 2001 , 63, 3-3	127

1938	Polarized absorption spectra of single-walled 4 Å carbon nanotubes aligned in channels of an AlPO ₄ (4-5) single crystal. 2001 , 87, 127401	263
1937	Density functional theory calculations of proton-containing defects in forsterite. 2001 , 154, 255-259	2
1936	The CO/Pt(111) Puzzle. 2001 , 105, 4018-4025	579
1935	Theoretical study of the ordered-vacancy semiconducting compound CdAl ₂ Se ₄ . 2001 , 13, 1669-1684	22
1934	Ab-initio simulation of isolated screw dislocations in bcc Mo and Ta. 2001 , 81, 1305-1316	105
1933	A First Principles Density Functional Study of Au Deposition on TiN (001) Surface. 2001 , 2, 263-270	6
1932	Ab-Initio Modeling of C-B Interactions In Si. 2001 , 669, 1	
1931	Modeling of Annealing of High Concentration Arsenic Profiles. 2001 , 669, 1	0
1930	Modeling Boron and Indium Electrical Activities in Silicon in the Presence of Nitrogen. 2001 , 669, 1	
1929	Simulations of long time scale dynamics using the dimer method. 2001 , 677, 811	4
1928	Multiscale Modeling of Stress-Mediated Diffusion in Silicon - Volume Tensors. 2001 , 677, 941	3
1927	Influence of magnetic interaction on lattice dynamics of FeBO ₃ . 2001 , 56, 275-281	15
1926	Stacking-fault energy and yield stress asymmetry in molybdenum disilicide. 2001 , 81, 1079-1097	17
1925	Ab initio study of graphite prismatic surfaces. 2001 , 177, 221-225	12
1924	The hydration number of Na ⁺ in liquid water. 2001 , 183-184, 121-132	121
1923	Photocatalytic TiO ₂ thin film deposited onto glass by DC magnetron sputtering. 2001 , 392, 338-344	285
1922	Nonmetal-metal transition in Ba _n clusters. 2001 , 117, 635-639	1
1921	Lattice dynamics of Mg ₂ SiO ₄ . 2001 , 596, 3-6	12

1920	Electron and atom dynamics at solid surfaces and relation to epitaxy. 2001 , 62, 1689-1730	9
1919	On the nature of RuS ₂ HDS active sites: insight from ab initio theory. 2001 , 174, 239-244	6
1918	Parallel between infrared characterisation and ab initio calculations of CO adsorption on sulphided Mo catalysts. 2001 , 70, 255-269	90
1917	Ab initio search of carbon nitrides, isoelectronic with diamond, likely to lead to new ultra hard materials. 2001 , 4, 255-272	5
1916	Theoretical Study of Possible Iridium Ditelluride Phases Attainable under High Pressure. 2001 , 162, 63-68	9
1915	Effects of oxidation on the nanoscale mechanisms of crack formation in aluminum. 2001 , 2, 55-9	36
1914	Existierende und hypothetische intermediäre AgII/AgIII- und AgII/AgI-Fluoride als potentielle Supraleiter. 2001 , 113, 2816-2859	26
1913	TlF and PbO under High Pressure: Unexpected Persistence of the Stereochemically Active Electron Pair. 2001 , 113, 4760-4765	8
1912	Real and Hypothetical Intermediate-Valence Ag /Ag and Ag /Ag Fluoride Systems as Potential Superconductors. 2001 , 40, 2742-2781	119
1911	TlF and PbO under High Pressure: Unexpected Persistence of the Stereochemically Active Electron Pair This work was supported by the Swedish National Science Research Council (NFR) and the Göran Gustafsson Foundation.. 2001 , 40, 4624-4629	22
1910	First-Principles Modeling of Boron Clustering in Silicon. 2001 , 226, 37-45	18
1909	Simulations of Molecular Fluids under Extreme Conditions. 2001 , 41, 139-142	3
1908	HARES: an efficient method for first-principles electronic structure calculations of complex systems. 2001 , 137, 341-360	35
1907	The role of adsorbates in the electrochemical oxidation of ammonia on noble and transition metal electrodes. 2001 , 506, 127-137	252
1906	Theoretical calculations of dissociative adsorption of CH ₄ on an Ir(111) surface. 2001 , 86, 664-7	124
1905	The phase diagram and electronic structure of Pd-V alloys: ab initio density functional calculations. 2001 , 13, 3545-3572	21
1904	First-principles prediction of structure, energetics, formation enthalpy, elastic constants, polarization, and piezoelectric constants of AlN, GaN, and InN: Comparison of local and gradient-corrected density-functional theory. <i>Physical Review B</i> , 2001 , 64,	3.3 366
1903	Structural, vibrational, and thermodynamic properties of Al-Sc alloys and intermetallic compounds. <i>Physical Review B</i> , 2001 , 64,	3.3 82

1902	Mechanism of hydrogen sorption in single-walled carbon nanotubes. 2001 , 123, 5845-6		115
1901	First-principles study of the atomic oxygen adsorption on the (0 0 0 1) graphite surface and dissolution. 2001 , 177, 226-229		26
1900	Crystal structure and stability of complex precipitate phases in AlCuMg(Si) and AlZnMg alloys. 2001 , 49, 3129-3142		334
1899	Structure Models for Aluminum Oxynitride from Ab Initio Calculations. 2001 , 84, 2633-2637		38
1898	Determination of solid-state sulfidation mechanisms in ion-implanted copper. 2001 , 175-177, 382-387		11
1897	Mechanical property degradation in irradiated materials: A multiscale modeling approach. 2001 , 180, 23-31		51
1896	Self-diffusion of adatoms on Ni(100) surfaces. 2001 , 13, L321-L328		18
1895	First Principles Study on Li Deintercalation Effect in Orthorhombic LiMnO ₂ . 2001 , 40, 6878-6883		1
1894	Parameter-free modelling of dislocation motion: The case of silicon. 2001 , 81, 1257-1281		60
1893	Restricting dislocation movement in transition metal carbides by phase stability tuning. 2001 , 293, 2434-7		92
1892	MgB ₂ under pressure: phonon calculations, Raman spectroscopy, and optical reflectance. 2001 , 13, 9945-9962		60
1891	Near-Edge X-ray Absorption Spectra of Carbon-Nitride Molecules and Solids. 2001 , 63, 70-86		16
1890	Elastic reversal of electrostatically driven defect ordering in stabilized zirconia. 2001 , 56, 393-399		13
1889	Surface structures by direct transform of electron diffraction patterns. 2001 , 13, 10709-10728		
1888	Theory of Sb-induced triple-period ordering in GaInP. <i>Physical Review B</i> , 2001 , 64,	3-3	11
1887	Vibrational modes in epitaxial Ti _{1-x} Sc _x N(001) layers: An ab initio calculation and Raman spectroscopy study. <i>Physical Review B</i> , 2001 , 64,	3-3	45
1886	First-principles study of Ca ²⁺ and Mn ²⁺ substituents in KTaO ₃ . <i>Physical Review B</i> , 2001 , 63,	3-3	22
1885	Transition-metal ion impurities in KTaO ₃ . <i>Physical Review B</i> , 2001 , 65,	3-3	24

1884	Diffusion kinetics in the Pd/Cu(001) surface alloy. 2001 , 86, 4588-91		72
1883	Density-functional theory calculations of the interaction of protons and water with low-coordinated surface sites of calcium oxide. <i>Physical Review B</i> , 2001 , 63,	3-3	35
1882	First principles investigation of scaling trends of zirconium silicate interface band offsets. 2001 , 90, 1333-1341		27
1881	Structure and interaction mechanism in the magic Al ₁₃ +H ₂ O cluster. 2001 , 64,		10
1880	Stability of a nonequilibrium phase in an immiscible Ag-Ni system studied by ab initio calculations and ion-beam-mixing experiment. <i>Physical Review B</i> , 2001 , 63,	3-3	24
1879	Structure of aluminum atomic chains. <i>Physical Review B</i> , 2001 , 64,	3-3	58
1878	Real-space representation of electron localization and shell structure in jelliumlike clusters. <i>Physical Review B</i> , 2001 , 63,	3-3	28
1877	Transition-metal interactions in aluminum-rich intermetallics. <i>Physical Review B</i> , 2001 , 64,	3-3	22
1876	Migration of O vacancies in β -quartz: The effect of excitons and electron holes. <i>Physical Review B</i> , 2001 , 64,	3-3	35
1875	Patterning of Si(001) with halogens: Surface structure as a function of the halogen chemical potential. <i>Physical Review B</i> , 2001 , 64,	3-3	22
1874	Adhesion of ultrathin ZrO ₂ (111) films on Ni(111) from first principles. 2001 , 114, 5816-5831		107
1873	Comparative dielectric response in CaTiO ₃ and CaAl _{1/2} Nb _{1/2} O ₃ from first principles. 2001 , 90, 1459-1468		24
1872	Te covered Si(001): A variable surface reconstruction. <i>Physical Review B</i> , 2001 , 64,	3-3	6
1871	Thermal fluctuations, localization, and self-trapping in a polar crystal: Combined shell-model molecular dynamics and quantum chemical approach. <i>Physical Review B</i> , 2001 , 64,	3-3	20
1870	Towards 100% spin-polarized charge-injection: The half-metallic NiMnSb/CdS interface. <i>Physical Review B</i> , 2001 , 64,	3-3	166
1869	Geometric and electronic structure of PdMn bimetallic systems on Pd(100). <i>Physical Review B</i> , 2001 , 65,	3-3	11
1868	Irradiation and interface induced formation of a nonequilibrium Ag ₃ Co phase predicted by ab initio calculation. <i>Physical Review B</i> , 2001 , 64,	3-3	22
1867	Density-functional calculation of multiple-shock Hugoniot of liquid nitrogen. <i>Physical Review B</i> , 2001 , 65,	3-3	25

1866	The competition between chemical bonding and magnetism in the adsorption of atomic Ni on MgO(100). 2001 , 115, 8172-8177		47
1865	Calculation of a deuterium double shock Hugoniot from ab initio simulations. 2001 , 87, 275502		86
1864	Ab initio studies of high-pressure transformations in GeO ₂ . <i>Physical Review B</i> , 2001 , 63,	3-3	49
1863	Thermodynamics of uniaxial phase transition: Ab initio study of the diamond-to-graphite transition in Si and Ge. <i>Physical Review B</i> , 2001 , 63,	3-3	22
1862	Neglected adsorbate interactions behind diffusion prefactor anomalies on metals. <i>Physical Review B</i> , 2001 , 64,	3-3	64
1861	An experimental and theoretical investigation of the thiophene/aluminum interface. 2001 , 114, 935		26
1860	Role of stress in thin film alloy thermodynamics: competition between alloying and dislocation formation. 2001 , 86, 660-3		50
1859	Surface relaxations, current enhancements, and absolute distances in high resolution scanning tunneling microscopy. 2001 , 87, 236104		101
1858	Structure of the Ba-induced Si(111)-(3 x 2) reconstruction. 2001 , 87, 056104		61
1857	Surface-diffusion mechanism versus electric field: Pt/Pt(001). <i>Physical Review B</i> , 2001 , 64,	3-3	80
1856	Structure determination of the Si ₃ N ₄ /Si(111)-(8 x 8) surface: a combined study of Kikuchi electron holography, scanning tunneling microscopy, and ab initio calculations. 2001 , 86, 2818-21		55
1855	The role of the nanoscale in surface reactions: CO ₂ on CdSe. 2002 , 89, 075506		19
1854	Strain-driven mesoscopic reconstruction of the As/Ge(111) surface. 2002 , 89, 076103		7
1853	Vibrational recognition of hydrogen-bonded water networks on a metal surface. 2002 , 89, 176104		207
1852	Critical role of the surface reconstruction in the thermodynamic stability of (105) Ge pyramids on Si(001). 2002 , 88, 256103		101
1851	Comprehensive ab initio thermodynamic treatment of impurities in ordered alloys: application to boron in B ₂ Fe-Al. 2002 , 89, 225502		14
1850	Surface model and exchange-correlation functional effects on the description of Pd/graphene-Al ₂ O ₃ (0001). 2002 , 116, 1684-1691		44
1849	Energetics of transition-metal ions in low-coordination environments. <i>Physical Review B</i> , 2002 , 66,	3-3	2

1848	First-principles calculation of the phonon spectrum of MgAl ₂ O ₄ spinel. <i>Physical Review B</i> , 2002 , 65,	3-3	56
1847	Crystal structure and lattice dynamics of AlB ₂ under pressure and implications for MgB ₂ . <i>Physical Review B</i> , 2002 , 66,	3-3	58
1846	Ab initio calculations for bromine adlayers on the Ag(100) and Au(100) surfaces: The c(2×) structure. <i>Physical Review B</i> , 2002 , 65,	3-3	24
1845	Chemical design of direct-gap light-emitting silicon. 2002 , 89, 076802		14
1844	Energetics of the dihydride phases on the diamond (100) surface. <i>Physical Review B</i> , 2002 , 65,	3-3	7
1843	Vibrational properties of tin clathrate materials. <i>Physical Review B</i> , 2002 , 65,	3-3	31
1842	Density-functional investigation of magnetism in UPu. <i>Physical Review B</i> , 2002 , 66,	3-3	118
1841	Interaction of Pd with Al ₂ O ₃ (0001): A case study of modeling the metal-oxide interface on complex substrates. <i>Physical Review B</i> , 2002 , 65,	3-3	50
1840	First-principles calculations of the adsorption, diffusion, and dissociation of a CO molecule on the Fe(100) surface. <i>Physical Review B</i> , 2002 , 66,	3-3	103
1839	Efficient Eley-Rideal reactions of H atoms with single Cl adsorbates on Au(111). 2002 , 89, 268302		30
1838	Stability of elongated and compact types of structures in SiO ₂ nanoparticles. <i>Physical Review B</i> , 2002 , 65,	3-3	36
1837	Self-diffusion rates in Al from combined first-principles and model-potential calculations. 2002 , 89, 065901		60
1836	Low-energy linear structures in dense oxygen: implications for the epsilon phase. 2002 , 88, 205503		56
1835	Initial stage of carbon incorporation into si(001) and one-dimensional ordering of embedded carbon. 2002 , 89, 106102		29
1834	Linking surface stress to surface structure: measurement of atomic strain in a surface alloy using scanning tunneling microscopy. 2002 , 89, 036101		33
1833	Atomic and electronic properties of anion vacancies on the (110) surfaces of InP, InAs, and InSb. <i>Physical Review B</i> , 2002 , 66,	3-3	16
1832	Instability of metallic In _n dimer lines on Si(100) 2× surface. <i>Physical Review B</i> , 2002 , 65,	3-3	11
1831	Complex band structure, decay lengths, and Fermi level alignment in simple molecular electronic systems. <i>Physical Review B</i> , 2002 , 65,	3-3	214

1830	Electronic states of prototype supertetrahedral framework materials. <i>Physical Review B</i> , 2002 , 66,	3-3	1
1829	First principles study of Pt adhesion and growth on SrO- and TiO ₂ -terminated SrTiO ₃ (100). 2002 , 116, 9914-9925		69
1828	SrTiO ₃ /MgO(001) and MgO/SrTiO ₃ (001) systems: Energetics and stresses. <i>Physical Review B</i> , 2002 , 66,	3-3	13
1827	Raman scattering study of stoichiometric Si and Ge type II clathrates. 2002 , 92, 7225-7230		51
1826	Importance of open-shell effects in adhesion at metal-ceramic interfaces. <i>Physical Review B</i> , 2002 , 66,	3-3	26
1825	Reconstruction and energetics of the polar (112) and (1 $\bar{1}$ 1 $\bar{2}$) versus the nonpolar (220) surfaces of CuInSe ₂ . <i>Physical Review B</i> , 2002 , 65,	3-3	82
1824	Interaction of HOCl with a chlorinated ice surface to produce molecular chlorine: An ab-initio study. 2002 , 116, 9856-9864		20
1823	Classical dynamics of dissociative adsorption for a nonactivated system: The role of zero point energy. 2002 , 116, 9005-9013		85
1822	Structure and bonding of propyne on Cu(111) from density functional periodic and cluster models. 2002 , 116, 1165-1170		17
1821	Atomistic modeling of solid-state amorphization in an immiscible Cu-Ta system. <i>Physical Review B</i> , 2002 , 66,	3-3	50
1820	First-principles calculation of Li adatom structures on the Mo(112) surface. <i>Physical Review B</i> , 2002 , 66,	3-3	29
1819	Density-functional theory investigation of hardness, stability, and electron-energy-loss spectra of carbon nitrides with C ₁₁ N ₄ stoichiometry. <i>Physical Review B</i> , 2002 , 65,	3-3	83
1818	Structural and magnetic properties of Fe/ZnSe(001) interfaces. <i>Physical Review B</i> , 2002 , 65,	3-3	10
1817	Self-interstitial trapping by carbon complexes in crystalline silicon. <i>Physical Review B</i> , 2002 , 66,	3-3	42
1816	Pt ₈₀ Fe ₂₀ surface from first principles: Electronic structure and adsorption of CO and atomic H. <i>Physical Review B</i> , 2002 , 66,	3-3	26
1815	Self-diffusion on fcc (100) metal surfaces: Comparison of different approximations. <i>Physical Review B</i> , 2002 , 65,	3-3	14
1814	Structural determination of two-dimensional YSi ₂ epitaxially grown on Si(111). <i>Physical Review B</i> , 2002 , 66,	3-3	24
1813	Formation of an ordered Si dimer structure on HfB ₂ (0001). <i>Physical Review B</i> , 2002 , 66,	3-3	9

1812	Properties of 4L carbon nanotubes from first-principles calculations. <i>Physical Review B</i> , 2002 , 66,	3-3	174
1811	Structural and superconducting transitions in Mg _{1-x} Al _x B ₂ . <i>Physical Review B</i> , 2002 , 66,	3-3	18
1810	Structures, energetics, and effects of stacking faults in MgB ₂ . <i>Physical Review B</i> , 2002 , 66,	3-3	8
1809	Optical Absorption of Large Band-Gap Sb _x Bi _{1-x} Al ₃ Alloys. 2002 , 744, 1		1
1808	Multiscale simulation of diffusion, deactivation, and segregation of dopants - ab-initio to continuum.		
1807	PERIODIC DFT STUDY OF ISOMORPHOUS INCORPORATION OF A V ION INTO (100) AND (001) ANATASE SURFACE LAYERS. 2002 , 09, 1425-1430		7
1806	Comparative Hartree-Fock and density-functional theory study of cubic and hexagonal diamond. 2002 , 82, 1767-1776		26
1805	Structure of Hydrated Microporous Aluminophosphates: Static and Molecular Dynamics Approaches of AlPO ₄ -34 from First Principles Calculations. 2002 , 106, 8599-8608		31
1804	Activation of group III combinations in silicon and modifications introduced by nitrogen. 2002 , 20, 230		6
1803	Magnetic properties of 3d impurities substituted in GaAs. 2002 , 14, 3295-3302		13
1802	Novel Bismuth Nanotubes. 2002 , 19, 1785-1787		4
1801	The viscosity of dense hydrogen: from liquid to plasma behaviour. 2002 , 14, 9089-9097		6
1800	Phase stability and pressure-induced semiconductor to metal transition in crystalline GeSe ₂ . 2002 , 14, 9589-9600		8
1799	Prediction of Possible Metastable Alloy Phases in an Equilibrium Immiscible YMo System by ab initio Calculation. 2002 , 17, 528-531		3
1798	Comparative study of nonequilibrium phase of A ₃ B and AB ₃ types in the NiMo system by first principles and thermodynamic calculations. 2002 , 17, 2720-2726		2
1797	Modeling Copper Diffusion in Silicon Oxide, Nitride, and Carbide. 2002 , 716, 841		4
1796	Enhanced polarization in strained BaTiO ₃ from first principles. 2002 , 718, 1		11
1795	Metastable Phase Formation in the Immiscible RuPd System Studied by Ab Initio Calculation and Ion Mixing. 2002 , 71, 2933-2935		2

1794	Ab initio Calculation to Predict Possible Non-Equilibrium Solid Phases in an Immiscible Y-Nb System. 2002 , 71, 141-143	13
1793	The Electronic Structure and other Properties of Amorphous Silicon Nitride Investigated with Density Functional Theory. 2002 , 715, 1011	3
1792	Ab-initio Calculations to Model Anomalous Fluorine Behavior. 2002 , 717, 1	10
1791	Ab-Initio Pseudopotential Calculations of Phosphorus Diffusion in Silicon. 2002 , 717, 1	
1790	Low Temperature Photoluminescence Studies of Narrow Bandgap GaAs Quantum Wells on GaAs. 2002 , 744, 1	
1789	First-principles Study of Electronic and Dielectric Properties of ZrO ₂ and HfO ₂ . 2002 , 745, 721/T5.2.1	4
1788	Oxygen vacancy defects in tantalum pentoxide: a density functional study. 2002 , 745, 761/T5.6.1	
1787	First-principles Study of Electronic and Dielectric Properties of ZrO ₂ and HfO ₂ . 2002 , 747, 1	
1786	Oxygen vacancy defects in tantalum pentoxide: a density functional study. 2002 , 747, 1	
1785	First-Principles Study of Atomic and Electronic Structure of Ba/Si(111). 2002 , 71, 2761-2764	6
1784	Oxides, Silicides, and Silicates of Zirconium and Hafnium; Density Functional Theory Study. 2002 , 716, 651	
1783	A DFT-Study of Structure and properties of Amorphous SiCN. 2002 , 731, 321	1
1782	First-Principles Simulation of Hydrogen Interaction in Amorphous Silicon Nitride. 2002 , 719, 8371	1
1781	Comparative study of the high-pressure behavior of As, Sb, and Bi. 2002 , 124, 15359-67	57
1780	Direct Dynamics Studies of CO-Assisted Carbon Nanotube Growth. 2002 , 106, 12418-12425	14
1779	Periodic Density Functional Theory Study of the Dissociative Adsorption of Molecular Oxygen over La ₂ O ₃ . 2002 , 106, 6543-6547	42
1778	Ab Initio Studies on the Thermal Dissociation Channels of cis- and trans-Azomethane. 2002 , 106, 6792-6801	8
1777	Dimensional changes as a function of charge injection for trans-polyacetylene: A density functional theory study. 2002 , 117, 7691-7697	19

1776	Density Functional Study of Benzene Adsorption on Pt(111). 2002 , 106, 7489-7498		147
1775	A First Principles Study of Carbon-Carbon Coupling over the {0001} Surfaces of Co and Ru. 2002 , 106, 2826-2829		64
1774	Density Functional Theory Calculations of Solid Solutions of Fluor- and Chlorapatites. 2002 , 14, 435-441		18
1773	Adsorption of Pyridine on the Gold(111) Surface: Implications for Alligator Clips for Molecular Wires. 2002 , 106, 6740-6747		101
1772	First Principles Calculations of the Adsorption Properties of CO and NO on the Defective TiO ₂ (110) Surface. 2002 , 106, 6184-6199		61
1771	Ab initio studies on Al ⁽⁺⁾ (H ₂ O) _(n) , HA(OH ⁽⁺⁾)(H ₂ O) _(n-1) , and the size-dependent H ₂ elimination reaction. 2002 , 124, 10846-60		31
1770	Dimensional changes as a function of charge injection in single-walled carbon nanotubes. 2002 , 124, 15076-80		82
1769	From local adsorption stresses to chiral surfaces: (R,R)-tartaric acid on Ni(110). 2002 , 124, 503-10		169
1768	O/Ag(100) Surface: A Density Functional Study with Slab Model. 2002 , 106, 3662-3667		26
1767	Hydrogenation of Benzene on Ni(111) A DFT Study. 2002 , 106, 13299-13305		53
1766	Island shape selection in Pt(111) submonolayer homoepitaxy with or without CO as an adsorbate. 2002 , 89, 146103		22
1765	Temperature dependence of infrared-active phonons in CaTiO ₃ : A combined spectroscopic and first-principles study. <i>Physical Review B</i> , 2002 , 66,	3-3	52
1764	Ideal pure shear strength of aluminum and copper. 2002 , 298, 807-11		608
1763	Lattice dynamics of NiTi austenite, martensite, and R phase. <i>Physical Review B</i> , 2002 , 66,	3-3	71
1762	Bismuth nanotubes: potential semiconducting nanomaterials. 2002 , 13, 746-749		35
1761	Elasticity of (Mg,Fe)SiO ₃ -perovskite at high pressures. 2002 , 29, 34-1		78
1760	FIRST PRINCIPLES MOLECULAR DYNAMICS INVOLVING EXCITED STATES AND NONADIABATIC TRANSITIONS. 2002 , 01, 319-349		125
1759	First-principles study of the structure and lattice dielectric response of CaCu ₃ Ti ₄ O ₁₂ . <i>Physical Review B</i> , 2002 , 65,	3-3	301

1758	Periodic Density Functional Study of CO and OH Adsorption on PtRu Alloy Surfaces: Implications for CO Tolerant Fuel Cell Catalysts. 2002 , 106, 686-692		244
1757	Electrical conductivity for warm, dense aluminum plasmas and liquids. 2002 , 66, 025401		378
1756	A Periodic Density Functional Theory Study of the Dehydrogenation of Methanol over Pt(111). 2002 , 106, 2559-2568		221
1755	Talc under tension and compression: Spinodal instability, elasticity, and structure. 2002 , 107, ECV 2-1-ECV 2-10		22
1754	Adsorption of ammonia on the gold (111) surface. 2002 , 116, 8981-8987		103
1753	Bcc and Fcc transition metals and alloys: a central role for the Jahn-Teller effect in explaining their ideal and distorted structures. 2002 , 124, 4811-23		28
1752	Pyroelectric properties of Al(In)GaN/GaN hetero- and quantum well structures. 2002 , 14, 3399-3434		689
1751	Atomistic model of gallium. <i>Physical Review B</i> , 2002 , 66,	3.3	52
1750	Theoretical Study of the MoS ₂ (100) Surface: A Chemical Potential Analysis of Sulfur and Hydrogen Coverage. 2. Effect of the Total Pressure on Surface Stability. 2002 , 106, 5659-5667		98
1749	The Effects of Lattice Motion on Eley-Rideal and Hot Atom Reactions: Quasiclassical Studies of Hydrogen Recombination on Ni(100) 2002 , 106, 8342-8348		28
1748	Electronic Structure of Chemically-Delithiated LiCoO ₂ Studied by Electron Energy-Loss Spectrometry. 2002 , 106, 1286-1289		83
1747	Simulation of growth of Cu on Ag(001) at experimental deposition rates. <i>Physical Review B</i> , 2002 , 66,	3.3	50
1746	First-principles study of the stability and electronic structure of metal hydrides. <i>Physical Review B</i> , 2002 , 66,	3.3	167
1745	Calculating the vacancy formation energy in metals: Pt, Pd, and Mo. <i>Physical Review B</i> , 2002 , 66,	3.3	161
1744	The s-p bonded representatives of the prominent BaAl ₄ structure type: a case study on structural stability of polar intermetallic network structures. 2002 , 124, 4371-83		75
1743	Bonding and stability of the hydrogen storage material Mg(2)NiH(4). 2002 , 41, 3684-92		79
1742	Graphite-like surface reconstructions on C{111} and their implication for n-type diamond. <i>Physical Review B</i> , 2002 , 66,	3.3	19
1741	Quantum transport through one-dimensional aluminum wires. 2002 , 20, 812		6

1740	First Principles Study of Cu Atoms Deposited on the β -Al ₂ O ₃ (0001) Surface. 2002 , 106, 11495-11500	31
1739	Hydrogen Stabilization of {111} Nanodiamond. 2002 , 740, 1	1
1738	Crystal structure and chemical bonding of the high-pressure phase of MgAl ₂ O ₄ from first-principles calculations. 2002 , 82, 2885-2894	2
1737	Thermodynamic stability of high-K dielectric metal oxides ZrO ₂ and HfO ₂ in contact with Si and SiO ₂ . 2002 , 80, 1897-1899	316
1736	Self-compensation in manganese-doped ferromagnetic semiconductors. 2002 , 89, 227201	150
1735	Pressure-induced structural transitions in MgH ₂ . 2002 , 89, 175506	160
1734	Periodic ab initio study of the hydrogenated rutile TiO ₂ (110) surface. 2002 , 497, 194-204	92
1733	First-principles study of the structural and energetic properties of H atoms on a graphite (0001) surface. 2002 , 496, 318-330	277
1732	Superstructures of carbon on V(). 2002 , 497, 294-304	10
1731	First-principles study of PdV surface alloys I. Electronic structure of clean surfaces. 2002 , 498, 21-36	22
1730	First-principles study of PdV surface alloys: II. Chemical reactivity. 2002 , 498, 37-52	17
1729	Tip effects in scanning tunneling microscopy of atomic-scale magnetic structures. 2002 , 498, L65-L70	11
1728	First-principles study of metallic iron interfaces. 2002 , 501, 261-269	51
1727	NO pairing and transformation to N ₂ O on Cu(111) and Pt(111) from first principles. 2002 , 506, L237-L242	55
1726	Ab initio molecular dynamics: recent progresses and limitations. 2002 , 312-314, 52-59	21
1725	Synthesis, structure determination, and quantum-chemical characterization of an alternate HgNCN polymorph. 2002 , 41, 4259-65	53
1724	Quantum-based atomistic simulation of materials properties in transition metals. 2002 , 14, 2825-2857	123
1723	First-principles electronic structure calculations of BaSi ₇ N ₁₀ with both corner- and edge-sharing SiN ₄ tetrahedra. 2002 , 336, 1-4	12

1722	Correlation of lattice constant versus tungsten concentration of the Ni-based solid solution examined by molecular dynamics simulation. 2002 , 337, 143-147	24
1721	Theoretical and experimental investigation of the electronic structure of Ti ₂ CrNi and Ti ₂ CrNi:H alloys. 2002 , 342, 337-342	15
1720	Flexible Ab initio boundary conditions: simulating isolated dislocations in bcc Mo and Ta. 2002 , 88, 216402	202
1719	Phonon spectrum of ZnAl ₂ O ₄ spinel from inelastic neutron scattering and first-principles calculations. <i>Physical Review B</i> , 2002 , 66,	3-3 49
1718	Partial dissociation of water on Ru(0001). 2002 , 295, 99-102	422
1717	An Atomic Perspective of a Doped Metal-Oxide Interface□□ 2002 , 106, 7995-8004	26
1716	Thermoelastic Properties of (Mg,Fe)SiO ₃ Perovskite. 2002 , 718, 1	
1715	Modeling Boron Diffusion in Polycrystalline HfO ₂ Films. 2002 , 716, 441	
1714	Ab-Initio Modeling of Boron and Oxygen Diffusion in Polycrystalline HfO ₂ Films. 2002 , 233, 18-23	7
1713	Theoretical Studies of Self-Diffusion and Dopant Clustering in Semiconductors. 2002 , 233, 24-30	18
1712	Nonlinear Behavior of Spontaneous and Piezoelectric Polarization in III-V Nitride Alloys. 2002 , 190, 65-73	39
1711	FeGa ₃ and RuGa ₃ : Semiconducting Intermetallic Compounds. 2002 , 165, 94-99	92
1710	Polymorphism of IrSn ₄ . 2002 , 168, 34-40	18
1709	Incorporating first-principles energetics in computational thermodynamics approaches. 2002 , 50, 2187-2197	83
1708	Structure and stability of hcp bulk and nano-precipitated Ag ₂ Al. 2002 , 50, 2443-2459	31
1707	The connection between ab initio calculations and interface adhesion measurements on metal/oxide systems: Ni/Al ₂ O ₃ and Cu/Al ₂ O ₃ . 2002 , 50, 3803-3816	190
1706	Modelling molecular vibrations in extended hydrogen-bonded networks □ crystalline bases of RNA and DNA and the nucleosides. 2002 , 280, 53-70	30
1705	Molecular deformations of halogeno-mesitylenes in the crystal: structure, methyl group rotational tunneling, and numerical modeling. 2002 , 285, 299-308	12

1704	Theoretical investigation of the Ziegler-Natta catalysis in heterogeneous conditions. 2002 , 89, 389-396	7
1703	Liquid metal embrittlement of the martensitic steel 91: influence of the chemical composition of the liquid metal.: Experiments and electronic structure calculations. 2002 , 301, 70-76	51
1702	Metastable states in an equilibrium immiscible Ni-Bu system studied by ab initio calculation and ion mixing experiment. 2002 , 121, 375-379	1
1701	High pressure elastic properties of solid argon from first-principles density functional and quasi-harmonic lattice dynamic calculations. 2002 , 122, 557-560	6
1700	Adsorption and reaction of thiophene on β -Mo ₂ C(0001). 2002 , 511, 294-302	42
1699	Full-coverage adsorption of water on SnO ₂ (0): the stabilisation of the molecular species. 2002 , 512, 29-36	27
1698	Surface relaxation and surface stress of Au(111). 2002 , 513, 263-271	53
1697	First principles calculations for electronic band structure of single-walled carbon nanotube under uniaxial strain. 2002 , 514, 222-226	37
1696	Acetylene molecules on the Si(0) surface: room-temperature adsorption and structural modification upon annealing. 2002 , 514, 376-382	22
1695	The structure of the oxygen-induced c(6 \times 6) reconstruction of V(1 1 0). 2002 , 512, 16-28	13
1694	Reconstructions of strongly reduced SnO ₂ (1 1 0) studied by first-principles methods. 2002 , 513, 26-36	52
1693	Scanning tunneling spectroscopy on clean and contaminated V(0). 2002 , 513, 9-25	13
1692	Density-functional theory studies of pyrite FeS ₂ (100) and (110) surfaces. 2002 , 513, 511-524	121
1691	Effect of oxide vacancies on metal island nucleation. 2002 , 515, L481-L486	87
1690	Finite temperature studies of Te adsorption on Si(001). 2002 , 519, 79-89	18
1689	Computing accurate surface energies and the importance of electron self-energy in metal/metal-oxide adhesion. 2002 , 520, L611-L618	84
1688	Theoretical study of the structure of propene adsorbed on Pt(0). 2002 , 519, 250-258	23
1687	Density-functional theory studies of pyrite FeS ₂ (0) and (0) surfaces. 2002 , 520, 111-119	65

1686	A tool for the interactive 3D visualization of electronic structure in molecules and solids. 2002 , 26, 313-9	44
1685	The structure and chemistry of the TiO(2)-rich surface of SrTiO(3) (001). 2002 , 419, 55-8	310
1684	Thin Ta films: growth, stability, and diffusion studied by molecular-dynamics simulations. 2002 , 413, 110-120	23
1683	Quantum-chemical calculations of CO and OH interacting with bimetallic surfaces. 2002 , 47, 3621-3628	179
1682	The mechanisms of the thermal decomposition of 5-nitro-1-hydrogen-tetrazole: ab initio MD and quantum chemistry studies. 2002 , 351, 459-468	4
1681	Tuning in on single molecular states: adsorption sites and STM images of maleic anhydride on Si(100). 2002 , 355, 347-354	21
1680	Ab initio and transition state theory studies of the energetics of H atom resurfacing on Ni(111). 2002 , 357, 389-396	16
1679	Correlation of adsorption energy with surface structure: ethylene adsorption on Pd surfaces. 2002 , 358, 377-382	58
1678	The adsorption of molecular oxygen on neutral and negative Aun clusters (n=2B). 2002 , 359, 493-499	190
1677	Dispersion of vibrational modes in benzoic acid crystals. 2002 , 364, 34-38	35
1676	Electronic structure and STM images of self-assembled styrene lines on a Si(100) surface. 2002 , 365, 129-134	32
1675	Studies of rhodium nanoparticles using the first principles density functional theory calculations. 2002 , 366, 368-376	51
1674	Shape and Edge Sites Modifications of MoS2 Catalytic Nanoparticles Induced by Working Conditions: A Theoretical Study. 2002 , 207, 76-87	285
1673	Electrical conductivity of hot expanded aluminum: experimental measurements and ab initio calculations. 2002 , 66, 056412	52
1672	Periodic density functional theory study of methane activation over La(2)O(3): activity of O(2-), O(-), O(2)(2-), oxygen point defect, and Sr(2+)-doped surface sites. 2002 , 124, 8452-61	174
1671	Binding energies and electronic structures of adsorbed titanium chains on carbon nanotubes. <i>Physical Review B</i> , 2002 , 66,	3-3 100
1670	Structure of the (001) surface of alumina. 2002 , 117, 4509-4516	27
1669	Pentagonal nanowires: A first-principles study of the atomic and electronic structure. <i>Physical Review B</i> , 2002 , 65,	3-3 72

1668	Hydrogen activation on Mo-based sulfide catalysts, a periodic DFT study. 2002 , 124, 7084-95		155
1667	Collective and single particle diffusion on surfaces. 2002 , 51, 949-1078		455
1666	Spin-polarization in half-metals (invited). 2002 , 91, 8340		173
1665	Structural relaxation and relative stability of nanodiamond morphologies. 2003 , 12, 1867-1872		100
1664	Ab initio modelling of the stability of nanocrystalline diamond morphologies. 2003 , 83, 39-45		63
1663	Vacancy Formation on MoS ₂ Hydrodesulfurization Catalyst: DFT Study of the Mechanism. 2003 , 107, 4057-4064		122
1662	Ab initio modelling of band states in doped diamond. 2003 , 83, 1163-1174		25
1661	Elucidation by computer simulations of the CUS regeneration mechanism during HDS over MoS ₂ in combination with 35S experiments. 2003 , 29, 589-607		15
1660	Electrical conductivity of a strongly correlated aluminium plasma. 2003 , 36, 6033-6039		22
1659	Stress-induced defects in Sb ₂ Te ₃ . <i>Physical Review B</i> , 2003 , 68,	3-3	70
1658	Coexistence of bucky diamond with nanodiamond and fullerene carbon phases. <i>Physical Review B</i> , 2003 , 68,	3-3	100
1657	Electronic structure and origin of ferromagnetism in Ga _{1-x} Mn _x As semiconductors. 2003 , 340-342, 874-877		9
1656	Methanol at the water/platinum interface studied by ab initio molecular dynamics. 2003 , 544, L697-L702		28
1655	Function of subsurface boron on Si(0 0 1)-2 × 1: water adsorption. 2003 , 547, L882-L886		5
1654	A model study for the breaking of N ₂ from CN _x within DFT. 2003 , 5, 701-703		23
1653	Chemical pressure and hydrogen insertion effects in CeNiIn. 2003 , 5, 1385-1393		16
1652	Perspectives on the first principles elucidation and the design of active sites. 2003 , 216, 73-88		138
1651	Kinetic interpretation of catalytic activity patterns based on theoretical chemical descriptors. 2003 , 216, 63-72		146

1650	Adsorption of unsaturated aldehydes on the (111) surface of a PtBe alloy catalyst from first principles. 2003 , 217, 354-366	67
1649	Ab initio contribution to the study of complexes formed during dilute FeCu alloys radiation. 2003 , 202, 44-50	62
1648	The connection between the electronic structure and the properties of binderless tungsten carbides. 2003 , 21, 55-61	25
1647	Ab initio study of energy-level alignments in polymer-dye blends. 2003 , 381, 392-396	10
1646	Thermal excitation of CO on the (2 11) Pt {1 1 0} surface: a theoretical simulation of a variable-temperature STM contrast. 2003 , 382, 41-47	
1645	Surface energy anisotropy of iron surfaces by carbon adsorption. 2003 , 3, 457-460	23
1644	Structures and thermodynamic phase transitions for oxygen and silver oxide phases on Ag{1 1 1}. 2003 , 367, 344-350	109
1643	Defect structure for proton transport in a triflic acid monohydrate solid. 2003 , 368, 108-114	83
1642	Ionization of HCl and HF in ice: a periodic DFT study. 2003 , 369, 287-292	31
1641	Quasi-chemical study of Be ²⁺ (aq) speciation. 2003 , 371, 613-619	57
1640	Structure and electronic properties of new model dinitride systems: a density-functional study of CN ₂ , SiN ₂ , and GeN ₂ . 2003 , 373, 636-641	40
1639	Atomic understanding of strong nanometer-thin metal/alumina interfaces. 2003 , 544, L689-L696	15
1638	Adsorption of water molecules on the CdTe surface. 2003 , 545, 34-40	5
1637	Structure of Fe(310) studied by quantitative LEED analysis and pseudopotential DFT calculations. 2003 , 546, L808-L812	4
1636	A DFT periodic study of the vanadyl pyrophosphate (100) surface. 2003 , 547, 438-451	9
1635	A first principles analysis of CO oxidation over Pt and Pt _{66.7%} Ru _{33.3%} (111) surfaces. 2003 , 48, 3759-3773	106
1634	Defect-induced nonpolar-to-polar transition at the surface of CuInSe ₂ . 2003 , 64, 1547-1552	17
1633	Tin-magnesium substitution in Ir ₃ Sn ₇ structure and chemical bonding in Mg _x Ir ₃ Sn _{7-x} (x=0-0.67). 2003 , 173, 418-424	27

1632	Ground- and excited-state properties of inorganic solids from full-potential density-functional calculations. 2003 , 176, 338-374	9
1631	Pathways to metastable nitride structures. 2003 , 176, 530-537	62
1630	Quantum chemical contributions on the reactivity of solids. 2003 , 176, 575-586	1
1629	Vibrational spectroscopy using ab initio density-functional techniques. 2003 , 651-653, 3-17	24
1628	Chirality dependence of the energetics and electronic properties of Li-intercalated 4 π carbon nanotubes. 2003 , 125, 77-82	26
1627	Ab initio calculation to predict the possible nonequilibrium A3B and AB3 states in the CoMo system. 2003 , 125, 435-437	4
1626	Reactivity of a reduced metal oxide surface: hydrogen, water and carbon monoxide adsorption on oxygen defective rutile TiO ₂ (δ). 2003 , 524, 49-62	153
1625	Mechanisms of hole formation in metal-on-metal epitaxial systems: Rh/Ag(0 0 1). 2003 , 524, L89-L95	9
1624	A periodic model for the V ₂ O ₅ /TiO ₂ (anatase) catalyst. Stability of dimeric species. 2003 , 526, 297-308	50
1623	Platinum nanocrystals supported by silica, alumina and ceria: metal-support interaction due to high-temperature reduction in hydrogen. 2003 , 532-535, 276-280	53
1622	Characteristics of S adsorption on Pd vicinal surfaces. 2003 , 532-535, 154-159	5
1621	Hydrogen recombination on a mixed adsorption layer at saturation on a metal surface: H-(D+H) _{sat} +Ni(δ). 2003 , 529, 11-22	9
1620	Structure and reactivity of Pd doped Ag surfaces. 2003 , 529, 403-409	8
1619	Oxidation of graphite by atomic oxygen: a first-principles approach. 2003 , 537, 55-63	71
1618	A combined ab initio and atomistic simulation study of the surface and interfacial structures and energies of hydrated scheelite: introducing a CaWO ₄ potential model. 2003 , 531, 159-176	53
1617	Adsorption and diffusion of a Si adatom on the H/Si(δ) surface: comparison with the H/Si(δ) surface. 2003 , 530, 155-160	12
1616	Calculation of magnetic and structural properties of small CoRh clusters. 2003 , 532-535, 334-340	35
1615	Electric field effects on surface dynamics: Si ad-dimer diffusion and rotation on Si(δ). 2003 , 536, 121-129	20

1614	Thin Pt films on the polar SrTiO ₃ (111) surface: an experimental and theoretical study. 2003 , 537, 134-152	59
1613	The importance of Pb-vacancy attractions on diffusion in the Pb/Cu(001) surface alloy. 2003 , 538, 53-58	15
1612	Surface structure of cubic diamond nanowires. 2003 , 538, 204-210	21
1611	Dimer binding energies on fcc() metal surfaces. 2003 , 539, L560-L566	27
1610	DFT study of adsorption and dissociation of thiophene molecules on Ni(110). 2003 , 540, 474-490	34
1609	Adsorption of Au atoms on stoichiometric and reduced TiO ₂ (110) rutile surfaces: a first principles study. 2003 , 542, 72-80	83
1608	Relaxation of the (001) surface in binary Sc, Ti and V nitrides: a first principles density functional study. 2003 , 541, 217-224	15
1607	Mixed PbSi dimer chains on Si(100): a first-principles study. 2003 , 542, L649-L654	3
1606	Pt/ceria thin film model catalysts after high-temperature reduction: a (HR)TEM study. 2003 , 71, 71-76	21
1605	Performance of the Vienna ab initio simulation package (VASP) in chemical applications. 2003 , 624, 37-45	161
1604	QUASI: A general purpose implementation of the QM/MM approach and its application to problems in catalysis. 2003 , 632, 1-28	790
1603	The surface science of titanium dioxide. 2003 , 48, 53-229	6317
1602	Proton tunnelling in the hydrogen bonds of halogen-substituted derivatives of benzoic acid studied by NMR relaxometry: the case of large energy asymmetry. 2003 , 291, 41-52	34
1601	Ab initio calculation of magnetization density in La ₂ NiO ₄ . 2003 , 257, 235-238	4
1600	First-principles calculations of the dielectric properties of perovskite-type materials. 2003 , 23, 2375-2379	17
1599	Rattling guest atoms in Si, Ge, and Sn-based type-II clathrate materials. 2003 , 239, 26-34	27
1598	Electronics and sensors based on pyroelectric AlGaN/GaN heterostructures. 2003 , 1878-1907	56
1597	Ferromagnetic instabilities in atomically thin lithium and sodium wires. 2003 , 91, 239-244	18

1596	Interface structures of III-V semiconductor heterostructures. 2003 , 95, 561-571		4
1595	Exploiting Covalency to Enhance Metal-Oxide and Oxide-Oxide Adhesion at Heterogeneous Interfaces. 2003 , 86, 373-386		31
1594	First-Principles Calculations of Microdomain Models for Hexagonal Si ₅ AlON ₇ . 2003 , 86, 1956-1958		10
1593	Crystal structures and shape-memory behaviour of NiTi. 2003 , 2, 307-11		276
1592	Ferromagnetism above room temperature in bulk and transparent thin films of Mn-doped ZnO. 2003 , 2, 673-7		1568
1591	Local structure and electronic properties of BaTaO ₂ N with perovskite-type structure. 2003 , 64, 281-286		59
1590	In search of new candidates for ultra-hard materials: the ternary BC ₃ N ₃ stoichiometry. 2003 , 64, 1539-1545		14
1589	Ab initio calculation of intrinsic point defects in CuInSe ₂ . 2003 , 64, 1657-1663		46
1588	Challenges and errors: interpreting high resolution images in scanning tunneling microscopy. 2003 , 71, 147-183		135
1587	Oxygen vacancy defects in tantalum pentoxide: a density functional study. 2003 , 69, 190-194		15
1586	Ab initio calculations and INS measurements of phonons and molecular vibrations in a model peptide compound Urea. 2003 , 291, 53-60		37
1585	Metastable phase formation in an immiscible Cu-Ta system studied by ion-beam mixing, ab initio calculation, and molecular dynamics simulation. 2003 , 51, 3885-3893		17
1584	Lattice dielectric response of CdCu ₃ Ti ₄ O ₁₂ and CaCu ₃ Ti ₄ O ₁₂ from first principles. <i>Physical Review B</i> , 2003 , 67,	3-3	86
1583	Anomalous grain boundary physics in polycrystalline CuInSe ₂ : the existence of a hole barrier. 2003 , 91, 266401		280
1582	Molecular alligator clips: a theoretical study of adsorption of S, Se and S ₈ on Au(111). 2003 , 14, 849-858		22
1581	Dynamic structure factor of liquid and amorphous Ge from ab initio simulations. <i>Physical Review B</i> , 2003 , 67,	3-3	33
1580	Comparison between plane-wave and linear-scaling localized basis sets for structural calculations of microporous molecular sieves. <i>Physical Review B</i> , 2003 , 68,	3-3	10
1579	New mechanism for the alpha to omega martensitic transformation in pure titanium. 2003 , 91, 025701		135

1578	Surface Coverage Effects on the Formation of Molecular Hydrogen on a Graphite Surface via an Eley-Rideal Mechanism. 2003 , 107, 10862-10871		19
1577	Surface structures of SrTiO ₃ (001): a TiO ₂ -rich reconstruction with a c(4 x 2) unit cell. 2003 , 125, 10050-6		120
1576	Size dependent phase stability of carbon nanoparticles: Nanodiamond versus fullerenes. 2003 , 118, 5094-509783		
1575	Adsorption of gold on stoichiometric and reduced rutile TiO ₂ (110) surfaces. 2003 , 118, 6536-6551		186
1574	Adsorption of Unsaturated Hydrocarbons on Pd(111) and Pt(111): A DFT Study. 2003 , 107, 12287-12295		129
1573	Structure of the P vacancy on the InP(110) surface from first principles. <i>Physical Review B</i> , 2003 , 67,	3-3	8
1572	Cubic Hf ₃ N ₄ and Zr ₃ N ₄ : A class of hard materials. <i>Physical Review B</i> , 2003 , 68,	3-3	242
1571	Force-based many-body interatomic potential for ZrC. 2003 , 93, 9072-9085		45
1570	Arsenic deactivation in Si: Electronic structure and charge states of vacancy-impurity clusters. <i>Physical Review B</i> , 2003 , 68,	3-3	68
1569	Magnetism of transition-metal/carbon-nanotube hybrid structures. 2003 , 90, 257203		195
1568	Structure of the icosahedral Ti-Zr-Ni quasicrystal. <i>Physical Review B</i> , 2003 , 67,	3-3	41
1567	First-principles calculations of intrinsic defects in Al ₂ O ₃ . <i>Physical Review B</i> , 2003 , 68,	3-3	244
1566	Spontaneous Cross Linking of Small-Diameter Single-Walled Carbon Nanotubes. 2003 , 3, 585-587		29
1565	Specific ethene surface activation on silver oxide covered Ag[111] from the interplay of STM experiment and theory. 2003 , 125, 3119-25		58
1564	Computer Modeling Study of the Effect of Hydration on the Stability of a Silica Nanotube. 2003 , 3, 1347-1352		51
1563	Free energy of liquid water on the basis of quasichemical theory and ab initio molecular dynamics. 2003 , 68, 041505		130
1562	Collective stabilization of hydrogen chemisorption on graphenic surfaces. <i>Physical Review B</i> , 2003 , 68,	3-3	62
1561	Density-Functional Study of the Adsorption and Vibration Spectra of Benzene Molecules on Pt(111). 2003 , 107, 2995-3002		106

- 1560 Ab Initio Modeling of Diamond Nanowire Structures. **2003**, 3, 1323-1328 68
- 1559 Adsorption Structures of Phenylacetylene and 1-Phenyl-1-propyne on a Si(100)-(2 × 1) Surface. **2003**, 107, 11987-11995 17
- 1558 Adsorption of HCl on Single-Crystal α -Al₂O₃ (0001) Surface: A DFT Study. **2003**, 107, 186-195 29
- 1557 Weakening of a Polyethylene Chain by Methyl Side Groups. **2003**, 1, 223-233 3
- 1556 Laves-phase structural changes in the system CaAl_{2-x}Mg_x. **2003**, 42, 1467-74 55
- 1555 Ab initio modelling of dopants in diamond nanowires: li. **2003**, 83, 2311-2321 4
- 1554 Crystal Structures of (Pyrene)₁₀(I₃-)4(I₂)₁₀ and [1,3,6,8-Tetrakis(methylthio)pyrene]₃(I₃-)3(I₂)₇: Structural Trends in Fused Aromatic Polyiodides. **2003**, 15, 1420-1433 23
- 1553 Ab initio study of phase transformations in boron nitride. *Physical Review B*, **2003**, 67, 3-3 95
- 1552 First-Principle Study of the Intercalation Process in the Li_xV₂O₅ System. **2003**, 15, 1812-1819 45
- 1551 Alloying effects on elastic properties of TiN-based nitrides. **2003**, 36, 2725-2729 117
- 1550 Structure and Energetics of Single-Walled Armchair and Zigzag Silicon Nanotubes. **2003**, 107, 7577-7581 79
- 1549 Structure and bonding of Sr₃In₁₁: how size and electronic effects determine structural stability of polar intermetallic compounds. **2003**, 42, 7782-8 28
- 1548 Atomistic Simulation of the Dissociative Adsorption of Water on Calcite Surfaces. **2003**, 107, 7676-7682 127
- 1547 Density Functional Theory Studies of Chemisorption and Diffusion Properties of Ni and Ni π thiophene Complexes on the MoS₂ Basal Plane. **2003**, 107, 1988-2000 15
- 1546 Spin crossover of spiro-biphenalenyl neutral radical molecular conductors. **2003**, 125, 13334-5 41
- 1545 Chemisorption of NO₂ on Carbon Nanotubes. **2003**, 107, 9363-9369 100
- 1544 First-Principles Calculations of the Adsorption of Nitromethane and 1,1-Diamino-2,2-dinitroethylene (FOX-7) Molecules on the Al(111) Surface. **2003**, 107, 8953-8964 37
- 1543 Ab initio investigations in magnetic oxides. **2003**, 31, 239-299 56

1542	Epitaxial BiFeO ₃ multiferroic thin film heterostructures. 2003 , 299, 1719-22		4944
1541	First-principles study of the structural energetics of PdTi and PtTi. <i>Physical Review B</i> , 2003 , 67,	3-3	31
1540	Theoretical study about adsorption of atomic oxygen on unmodified and I-modified Ag(100) surface. 2003 , 118, 11210-11216		5
1539	A Computer Modeling Study of Perfect and Defective Silver (111) Surfaces. 2003 , 107, 3528-3534		22
1538	Adsorption energy and spin state of first-row transition metals adsorbed on MgO(100). <i>Physical Review B</i> , 2003 , 67,	3-3	65
1537	Structure effects on the energetic, electronic, and magnetic properties of palladium nanoparticles. 2003 , 118, 5793-5801		65
1536	Anisotropy of the mobility of pentacene from frustration. 2003 , 139, 109-114		123
1535	Oxygen adsorption on Au clusters and a rough Au(111) surface: The role of surface flatness, electron confinement, excess electrons, and band gap. 2003 , 118, 4198-4205		240
1534	Electronic structure and ground states of transition metals encapsulated in a Si ₁₂ hexagonal prism cage. <i>Physical Review B</i> , 2003 , 68,	3-3	115
1533	Critical Size of the Phase Transition from Cubic to Tetragonal in Pure Zirconia Nanoparticles. 2003 , 3, 871-875		97
1532	Atomic scale computer aided design for novel semiconductor devices. 2003 , 27, 10-15		6
1531	Electronic structure of perovskite-type YBRh ₃ : X-ray photoelectron spectroscopy and ab initio band calculations. 2003 , 349, 206-210		2
1530	Electronic structure of magnesium nitride-fluorides from first-principles calculations. 2003 , 351, 72-76		22
1529	First principles study of sodiumAluminumHydrogen phases. 2003 , 356-357, 486-489		40
1528	Epitaxial ferromagnetic Mn ₅ Ge ₃ on Ge(111). 2003 , 83, 5002-5004		157
1527	Effects of the iron-oxide layer in Fe-FeO-MgO-Fe tunneling junctions. <i>Physical Review B</i> , 2003 , 68,	3-3	199
1526	First principles study of oxygen vacancy defects in tantalum pentoxide. 2003 , 94, 5609-5612		91
1525	Co-phase penetration of WC(101̄0)/WC(101̄0) grain boundaries from first principles. <i>Physical Review B</i> , 2003 , 67,	3-3	76

1524	Density-functional calculations of the liquid deuterium Hugoniot, reshock, and reverberation timing. <i>Physical Review B</i> , 2003 , 68,	3-3	156
1523	First-principles study of small-radius single-walled BN nanotubes. <i>Physical Review B</i> , 2003 , 68,	3-3	170
1522	Relationship between surface dipole, work function and charge transfer: Some exceptions to an established rule. <i>Physical Review B</i> , 2003 , 68,	3-3	283
1521	Electronic structure and magnetism of Mn-doped GaN. <i>Physical Review B</i> , 2003 , 68,	3-3	120
1520	Variations of the Geometries and Band Gaps of Single-Walled Carbon Nanotubes and the Effect of Charge Injection. 2003 , 107, 6924-6931		84
1519	Enhancement of electronic conductivity of LiFePO ₄ by Cr doping and its identification by first-principles calculations. <i>Physical Review B</i> , 2003 , 68,	3-3	219
1518	Magnetic and electronic structure of (Ga _{1-x} Mn _x)As. <i>Physical Review B</i> , 2003 , 67,	3-3	61
1517	Energetics and stability of nanostructured amorphous carbon. <i>Physical Review B</i> , 2003 , 67,	3-3	33
1516	First-principles study of adhesion at Cu/SiO ₂ interfaces. <i>Physical Review B</i> , 2003 , 68,	3-3	76
1515	Configurations, energies, and thermodynamics of the neutral MgH complex in GaN. 2003 , 94, 4918		16
1514	Self-doping of gold chains on silicon: a new structural model for Si(111)-(5 x 2)-Au. 2003 , 91, 206101		84
1513	Aluminum equation-of-state data in the warm dense matter regime. 2003 , 91, 075002		56
1512	Rietveld refinement and ab initio calculations of a C14-like Laves phase in Ti-Zr-Ni. 2003 , 83, 65-71		8
1511	Scanning tunneling microscopy and spectroscopy of gallium oxide deposition and oxidation on GaAs(001)-c(2x2)/(2x2). 2003 , 119, 6719-6728		136
1510	Equation of state and phonon frequency calculations of diamond at high pressures. <i>Physical Review B</i> , 2003 , 68,	3-3	69
1509	Melem (2,5,8-triamino-tri-s-triazine), an important intermediate during condensation of melamine rings to graphitic carbon nitride: synthesis, structure determination by X-ray powder diffractometry, solid-state NMR, and theoretical studies. 2003 , 125, 10288-300		805
1508	Theoretical evaluation of hydrogen storage capacity in pure carbon nanostructures. 2003 , 119, 2376-2385		232
1507	Water alignment and proton conduction inside carbon nanotubes. 2003 , 90, 195503		207

1506	Ideal tensile strength and band gap of single-walled carbon nanotubes. <i>Physical Review B</i> , 2003 , 68,	3.3	159
1505	Mg segregation at Al/Al ₃ Sc heterophase interfaces on an atomic scale: experiments and computations. 2003 , 91, 036101		79
1504	Steric Effects on the Adsorption of Alkylthiolate Self-Assembled Monolayers on Au (111) 2003 , 107, 3803-3807		70
1503	First-principles calculations of the adsorption of nitromethane and 1,1-diamino 2,2-dinitroethylene (FOX-7) molecules on the Al[111]surface.		1
1502	Nucleation of single-walled carbon nanotubes. 2003 , 90, 145501		121
1501	Pressure-induced phase of NaAlH ₄ : A potential candidate for hydrogen storage?. 2003 , 82, 2257-2259		107
1500	Ab initio modeling of B and N in C ₂₉ and C ₂₉ H ₂₄ nanodiamond. 2003 , 118, 10725-10728		20
1499	First-principles study of oxygen-vacancy pinning of domain walls in PbTiO ₃ . <i>Physical Review B</i> , 2003 , 68,	3.3	227
1498	Phonon DOS of filled skutterudite, Ba/sub 0.1/CoSb/sub 3/.		
1497	Cross-sectional scanning tunneling microscopy of Mn-doped GaAs: Theory and experiment. <i>Physical Review B</i> , 2003 , 68,	3.3	42
1496	Novel Method for the Activation of Acceptor Dopant in AlN Introducing Localized Band by Isoelectronic Dopant. 2003 , 798, 164		
1495	Theoretical Analysis of Oxygen Diffusion in monoclinic HfO ₂ . 2003 , 786, 541		7
1494	Modeling the polymorphism of pentacene. 2003 , 125, 6323-30		198
1493	Density Functional Theory Study of the Interaction of Cl ⁺ with Passivated Nickel Surfaces. 2003 , 6, B47		29
1492	Quadruple-period ordering in MBE GaAsSb alloys. 2003 , 794, 49		
1491	Influence of Stress on Thermoelectric Properties of Antimony Telluride. 2003 , 793, 38		
1490	Local Structural Variations in A ₁₇₂ M ₂₀ Co ₈ Decagonal Quasicrystals. 2003 , 805, 248		
1489	Order-disorder transition in the Cd-Ca cubic approximant. 2003 , 805, 50		3

1488	Ab-initio Study of the Diffusion Coefficients in Fe-based Liquids. 2003 , 806, 155		1
1487	Prediction of metastable phase formation in an immiscible CuCr system from interatomic potential and ab initio calculation. 2003 , 18, 2300-2303		3
1486	Quantum Molecular Dynamics calculations of radiative opacities. 2003 , 405, L5-L9		25
1485	Quasicrystal approximants with novel compositions and structures. 2003 , 805, 112		2
1484	Electronic versus geometric contrast in cross-sectional STM images of III-V semiconductor heterostructures. <i>Physical Review B</i> , 2003 , 67,	3-3	19
1483	Initial and final state effects in the x-ray absorption process of La _{1-x} Sr _x MnO ₃ . <i>Physical Review B</i> , 2003 , 68,	3-3	21
1482	Atomic and electronic structure of the Si/SrTiO ₃ interface. <i>Physical Review B</i> , 2003 , 68,	3-3	121
1481	Atomic structure and theoretical scanning tunneling microscopy images of Li zigzag chains on the GaAs(110) surface. <i>Physical Review B</i> , 2003 , 67,	3-3	2
1480	First-principles study of the role of solvent in the dissociation of water over a Pt-Ru alloy. <i>Physical Review B</i> , 2003 , 68,	3-3	77
1479	Bi incorporation in GaN and Al _x Ga _{1-x} N alloys. <i>Physical Review B</i> , 2003 , 68,	3-3	3
1478	Energetics and structural relaxation of constitutional defects in CoAl and CoTi from first principles. <i>Physical Review B</i> , 2003 , 68,	3-3	10
1477	Energetics of Li atom displacements in K _{1-x} Li _x TaO ₃ : First-principles calculations. <i>Physical Review B</i> , 2003 , 68,	3-3	37
1476	Solubility, diffusion, and precipitation of oxygen impurities in MgB ₂ . <i>Physical Review B</i> , 2003 , 67,	3-3	12
1475	Glass-forming ability determined by an n-body potential in a highly immiscible Cu-W system through molecular dynamics simulations. <i>Physical Review B</i> , 2003 , 68,	3-3	15
1474	Toward one-band superconductivity in MgB ₂ . <i>Physical Review B</i> , 2003 , 68,	3-3	79
1473	Ab initio valence band offsets between Si(100) and SiO ₂ from microscopic models. <i>Physical Review B</i> , 2003 , 67,	3-3	24
1472	Deep nitrogen-induced valence- and conduction-band states in GaAs _{1-x} N _x . <i>Physical Review B</i> , 2003 , 68,	3-3	20
1471	Quantum design and synthesis of a boron-oxygen-titanium phase. 2003 , 82, 4286-4288		1

1470	Nearest-neighbor configuration in (GaIn)(NAs) probed by x-ray absorption spectroscopy. 2003 , 90, 145505		112
1469	Mechanisms of molecular manipulation with the scanning tunneling microscope at room temperature: chlorobenzene/si(111)-(7 x 7). 2003 , 91, 118301		77
1468	Multiple time scale simulations of metal crystal growth reveal the importance of multiatom surface processes. 2003 , 90, 116101		78
1467	Hafnium nitride with thorium phosphide structure: physical properties and an assessment of the Hf-N, Zr-N, and Ti-N phase diagrams at high pressures and temperatures. 2003 , 90, 125501		149
1466	Ideal reactions of H atoms with Cl adsorbed on Au(111): Quantum and quasiclassical studies. 2003 , 118, 2357-2366		26
1465	Modeling the adsorption of norbornadiene on the Si(001) surface: The predominance of non-[2+2]-cycloaddition products. 2003 , 119, 1115-1126		11
1464	Theories of scanning probe microscopes at the atomic scale. 2003 , 75, 1287-1331		397
1463	Surface structure and dynamics of KTaO ₃ (001). <i>Physical Review B</i> , 2003 , 68,	3-3	10
1462	Nature and strength of defect interactions in cubic stabilized zirconia. <i>Physical Review B</i> , 2003 , 67,	3-3	92
1461	Diffusion of an adsorbed Si atom on the Si(111)(7x7) surface. <i>Physical Review B</i> , 2003 , 67,	3-3	32
1460	Surface structure and stability of PdZn and PtZn alloys: Density-functional slab model studies. <i>Physical Review B</i> , 2003 , 68,	3-3	94
1459	3x3 reconstruction of the Sm/Si(111) interface. <i>Physical Review B</i> , 2003 , 67,	3-3	25
1458	Dimensional change as a function of charge injection in graphite intercalation compounds: A density functional theory study. <i>Physical Review B</i> , 2003 , 68,	3-3	21
1457	Prediction of dopant ionization energies in silicon: The importance of strain. <i>Physical Review B</i> , 2003 , 68,	3-3	14
1456	Predicted hcp Ag-Al metastable phase diagram, equilibrium ground states, and precipitate structure. <i>Physical Review B</i> , 2003 , 67,	3-3	37
1455	Multilayer relaxation of Cu(210) studied by layer-doubling LEED analysis and pseudopotential density functional theory calculations. <i>Physical Review B</i> , 2003 , 68,	3-3	16
1454	Theoretical investigation of a possible Mn _x Si _{1-x} ferromagnetic semiconductor. <i>Physical Review B</i> , 2003 , 68,	3-3	42
1453	Ordered versus disordered growth of copper quantum wires on Mo and W vicinal surfaces. <i>Physical Review B</i> , 2003 , 67,	3-3	3

1452	Lattice dynamics of HgSe: Neutron scattering measurements and ab initio studies. <i>Physical Review B</i> , 2003 , 67,	3-3	21
1451	Predicted absence of ferromagnetism in manganese-doped diamond. <i>Physical Review B</i> , 2003 , 68,	3-3	27
1450	First-principles study on the energetics and vibrational properties of the S ₂ impurity in alkali-halide crystals. <i>Physical Review B</i> , 2003 , 68,	3-3	6
1449	Carbon nanotube bundles under high pressure: Transformation to low-symmetry structures. <i>Physical Review B</i> , 2003 , 68,	3-3	69
1448	Ab initio studies of stepped Pd surfaces with and without S. <i>Physical Review B</i> , 2003 , 67,	3-3	21
1447	Theoretical study of the ternary spinel nitride system Si ₃ N ₄ /Te ₃ N ₄ . <i>Physical Review B</i> , 2003 , 67,	3-3	37
1446	Vibrations of a water adlayer on Ru(0001). <i>Physical Review B</i> , 2003 , 67,	3-3	53
1445	Interactions and structure of poly(dimethylsiloxane) at silicon dioxide surfaces: Electronic structure and molecular dynamics studies. 2003 , 118, 5132-5142		56
1444	Theory of polarization enhancement in epitaxial BaTiO ₃ /SrTiO ₃ superlattices. 2003 , 82, 1586-1588		296
1443	Effect of composition on vacancy mediated diffusion in random binary alloys: First principles study of the Si _{1-x} Ge _x system. 2003 , 94, 174-185		37
1442	Tile Hamiltonian for decagonal AlCoCu derived from first principles. <i>Physical Review B</i> , 2003 , 67,	3-3	10
1441	Distance dependence of the interaction between single atoms: gold dimers on NiAl(110). 2003 , 90, 196103		76
1440	Quantum molecular-dynamics study of the electrical and optical properties of shocked liquid nitrogen. <i>Physical Review B</i> , 2003 , 67,	3-3	29
1439	Growth model for atomic ordering: the case for quadruple-period ordering in GaAsSb alloys. 2003 , 90, 026102		8
1438	Formation of the c(1×1) Cu monolayer on CaO(100): A theoretical study. <i>Physical Review B</i> , 2003 , 68,	3-3	5
1437	Ferromagnetic materials in the zinc-blende structure. <i>Physical Review B</i> , 2003 , 68,	3-3	123
1436	Theoretical study of laser characteristics of InPAsN/GaInAsP/InP laser diode using first-principles method.		
1435	Chemisorption of benzene and STM dehydrogenation products on Cu(100). <i>Physical Review B</i> , 2003 , 68,	3-3	76

1434	First-principles calculations of Fe on GaAs(100). <i>Physical Review B</i> , 2003 , 67,	3-3	61
1433	Layer spacings in coherently strained epitaxial metal films. 2003 , 90, 216105		34
1432	Nanocrystal formation and faceting instability in Al(110) homoepitaxy: true upward adatom diffusion at step edges and island corners. 2003 , 91, 016102		51
1431	Atomic structure of the Ba-induced Si(111)3 \times 3 reconstruction studied by LEED, STM, and ab initio calculations. <i>Physical Review B</i> , 2003 , 68,	3-3	23
1430	Displacement of surface arsenic atoms by insertion of oxygen atoms into AsGa backbonds. 2003 , 119, 9191-9198		10
1429	Atomic ordering in In _x Ga _{1-x} As alloy thin films: Action of surfactants. <i>Physical Review B</i> , 2003 , 68,	3-3	8
1428	Changing the diffusion mechanism of Ge-Si dimers on Si(001) using an electric field. 2003 , 91, 206104		14
1427	Uniaxial phase transition in Si: Ab initio calculations. <i>Physical Review B</i> , 2003 , 67,	3-3	16
1426	Ab initio studies of quasi-one-dimensional pentagon and hexagon ice nanotubes. 2003 , 118, 3913-3916		49
1425	Ab initio studies of the passive film formed on iron. <i>Physical Review B</i> , 2003 , 67,	3-3	22
1424	Ab initio study of elastic properties of Ir and Ir ₃ X compounds. 2003 , 93, 2414-2417		112
1423	Role of dynamic trapping in H ₂ dissociation and reflection on Pd surfaces. 2003 , 118, 11226-11234		63
1422	Theory of surfactant (Sb) induced reconstructions on InP(001). <i>Physical Review B</i> , 2003 , 67,	3-3	19
1421	Influence of sulfur on the adhesion of the nickel/alumina interface. <i>Physical Review B</i> , 2003 , 67,	3-3	75
1420	Random registry shifts in quasi-one-dimensional adsorbate systems. <i>Physical Review B</i> , 2003 , 67,	3-3	25
1419	Stability of Sb line structures on Si(001). <i>Physical Review B</i> , 2003 , 67,	3-3	16
1418	Reactive wetting: H ₂ O/Rh(111). 2003 , 90, 186103		39
1417	Comment on "vibrational recognition of hydrogen-bonded water networks on a metal surface". 2003 , 91, 059601; author reply 059602		35

1416	Observation of spin-polarized surface states on ultrathin bct Mn(001) films by spin-polarized scanning tunneling spectroscopy. 2003 , 90, 056803		87
1415	Vacancy-mediated and exchange diffusion in a Pb/Cu(111) surface alloy: concurrent diffusion on two length scales. 2003 , 90, 126102		41
1414	Geometry and electronic structure of β -Pu: A theoretical study. <i>Physical Review B</i> , 2003 , 68,	3-3	36
1413	Ab initio density functional studies of stepped TaC surfaces. <i>Physical Review B</i> , 2003 , 67,	3-3	5
1412	Six low-strain zinc-blende half metals: An ab initio investigation. <i>Physical Review B</i> , 2003 , 67,	3-3	166
1411	Electronic structure of Te- and As-covered Si(211). <i>Physical Review B</i> , 2003 , 68,	3-3	12
1410	Magnetic properties of Co and Co-Ag alloys in equilibrium/nonequilibrium structures studied by ab initio calculations. <i>Physical Review B</i> , 2003 , 68,	3-3	24
1409	Understanding ultrahigh doping: the case of boron in silicon. 2003 , 90, 026103		40
1408	Electronic and optical properties of β -layer GaN/(GaAs) $_n$ superlattices. <i>Physical Review B</i> , 2003 , 67,	3-3	
1407	First Principles Investigations of Diamond Ultrananocrystals. 2003 , 17, 3865-3879		24
1406	Hydrogenation of Nanodiamond Surfaces: Structure and Effects on Crystalline Stability. 2003 , 10, 233-239		23
1405	Ab initio modelling of boron and nitrogen in diamond nanowires. 2003 , 83, 2301-2309		7
1404	Quantum transport properties of ultrathin silver nanowires. 2003 , 14, 501-504		67
1403	Structural relaxations, vibrational dynamics and thermodynamics of vicinal surfaces. 2003 , 15, S3197-S3226		24
1402	Comparison of density functional theory methods as applied to compound semiconductor-oxide interfaces: Slab versus cluster models. 2003 , 21, 1908		9
1401	Electron confinement effects on Ni-based nanostructures. 2003 , 15, S2547-S2574		10
1400	Vibrational modes of three-membered self-interstitial clusters in silicon. 2003 , 15, 7851-7857		7
1399	First-principles molecular dynamics study of the stretching frequencies of hydrogen molecules in carbon nanotubes. 2003 , 5, 124-124		12

1398	Construction of an N-Body Cu-Ta Potential and Study of Interfacial Behavior between Immiscible Cu and Ta through Molecular Dynamics Simulation. 2003 , 72, 5-8	4
1397	Electrical and Optical Properties of Ultra-small Carbon Nanotubes Arrayed in Channels of Zeolite Single Crystals. 2003 , 44, 2066-2069	4
1396	Ideal and hot atom reactions between H atoms on metal and graphite surfaces. 2003 , 51-77	4
1395	Isotope velocity differentiation in thin carbon nanotubes through quantum diffusion. 2003 , 63, 254-260	3
1394	Construction of an Embedded-Atom Potential for an Immiscible Cu-V System. 2003 , 72, 464-467	3
1393	Electronic Structure Calculations of Phase Stability: Cohesive and Elastic Properties. 2003 , 1-11	2
1392	Formation Energies of Point Defects in Copper Indium Diselenide Using ab initio Methods. 2003 , 763, 8101	1
1391	Lattice Instabilities of Perovskite Oxides from First Principles. 2004 , 213-225	1
1390	Localization in an occupied-subspace-optimization approach to electronic structure: application to yttria-stabilized zirconia. 2004 , 12, 133-141	1
1389	Structural Stability and the Correlation of Lattice Constant versus Tantalum Concentration of the Ag-Based Fcc Solid Solutions Studied by Molecular Dynamics Simulation. 2004 , 43, 2589-2593	2
1388	An azanorbornadiene anchor for molecular-level construction on silicon(100). 2004 , 15, 324-332	22
1387	Ab initio molecular dynamics simulation on temperature-dependent properties of AlBi liquid alloy. 2004 , 16, 2507-2514	23
1386	Ab initio theory of magnetic interactions at surfaces. 2004 , 16, S2557-S2574	10
1385	First-principles study of binary transition-metal clusters and alloys. 2004 , 16, S2263-S2272	23
1384	Spin-polarized Shockley state at Ni(111) free surface and at Ni-Cu based structures on Cu(111) surface. 2004 , 67, 90-95	11
1383	Ab initio calculations of spin polarization at Co ₂ CrAl/GaAs interfaces. 2004 , 16, S5725-S5728	21
1382	Lattice vibrations and thermal properties of carbon nitride with defect ZnS structure from first-principles calculations. 2004 , 16, 3027-3034	6
1381	Comparative study of metastable phase formation in the immiscible Cu-W system by ab initio calculation and n-body potential. 2004 , 16, 5251-5258	14

1380	Nitrogen Adatom Diffusion on a Ga-Rich GaN (0001) Surface. 2004 , 21, 527-529		3
1379	The interstitial CiOi defect in bulk Si and Si1 'xGex. 2004 , 16, 8545-8555		5
1378	Atomic and Electronic Structures of Zr Atomic Chains. 2004 , 21, 1791-1794		8
1377	The pressure induced phase transition of confined water from ab initio molecular dynamics simulation. 2004 , 16, 8851-8859		2
1376	Comment on "Theoretical evaluation of hydrogen storage capacity in pure carbon nanostructures" [J. Chem. Phys. 119, 2376 (2003)]. 2004 , 120, 9427-9; author reply 9430-2		5
1375	Theoretical investigation of the valence-band offset between Si(001) and SiO2. <i>Physical Review B</i> , 2004 , 70,	3-3	23
1374	Comparison of predicted ferromagnetic tendencies of Mn substituting the Ga site in IIIIVB and in IIIIV2 chalcopyrite semiconductors. 2004 , 84, 3753-3755		30
1373	Stabilization of substitutional Mn in silicon-based semiconductors. <i>Physical Review B</i> , 2004 , 70,	3-3	38
1372	Electronic structure and ferromagnetism of Mn-substituted CuAlS2, CuGaS2, CuInS2, CuGaSe2, and CuGaTe2. <i>Physical Review B</i> , 2004 , 69,	3-3	43
1371	Electronic structure of crystalline binary and ternary CdTeD compounds. <i>Physical Review B</i> , 2004 , 70,	3-3	35
1370	Vibrational properties of the high-pressure Cmcm phase of ZnTe. <i>Physical Review B</i> , 2004 , 70,	3-3	13
1369	First-principles prediction of a decagonal quasicrystal containing boron. 2004 , 93, 095507		17
1368	Structure of ultrathin crystalline SiO2 films on Mo(112). <i>Physical Review B</i> , 2004 , 69,	3-3	27
1367	Relationship between domain-boundary free energy and the temperature dependence of stress-domain patterns of Pb on Cu(111). <i>Physical Review B</i> , 2004 , 70,	3-3	18
1366	Surface energetics and structure of the Ge wetting layer on Si(100). <i>Physical Review B</i> , 2004 , 70,	3-3	52
1365	Effect of chemical composition on the elastic and electrical properties of the boron-oxygen-yttrium system studied by ab initio and experimental means. <i>Physical Review B</i> , 2004 , 69,	3-3	1
1364	First-principles study of wurtzite-structure MnO. <i>Physical Review B</i> , 2004 , 70,	3-3	16
1363	Atomic and electronic structure of the KBi(111)3BR30°B chemisorption system. <i>Physical Review B</i> , 2004 , 70,	3-3	18

1362	Highly n-doped silicon: Deactivating defects of donors. <i>Physical Review B</i> , 2004 , 70,	3-3	30
1361	Molecular chemisorption as the theoretically preferred pathway for water adsorption on ideal rutile TiO ₂ (110). 2004 , 93, 086105		151
1360	When Langmuir is too simple: H ₂ dissociation on Pd(111) at high coverage. 2004 , 93, 146103		73
1359	Self-assembly via adsorbate-driven dislocation reactions. 2004 , 92, 106101		19
1358	Boron diffusion in strained Si: A first-principles study. 2004 , 96, 5543-5547		8
1357	Phosphine dissociation on the Si(001) surface. 2004 , 93, 226102		58
1356	Nucleation of Pd dimers at defect sites of the MgO(100) surface. 2004 , 92, 096105		98
1355	Experimental evidence for a partially dissociated water bilayer on Ru[0001]. 2004 , 93, 196102		119
1354	Carbon nanotubes-zeolite complex: A Li-intercalated compound with high storage capacity. 2004 , 84, 2649-2651		30
1353	Atomic force algorithms in density functional theory electronic-structure techniques based on local orbitals. 2004 , 121, 6186-94		32
1352	Atomic level scanning transmission electron microscopy characterization of GaN/AlN quantum wells. 2004 , 96, 738-746		10
1351	N vacancy diffusion and trapping in Mg-doped wurtzite GaN. 2004 , 96, 2015-2022		19
1350	Using polarity for engineering oxide nanostructures: structural phase diagram in free and supported MgO(111) ultrathin films. 2004 , 93, 215702		95
1349	Theory of hydrogen-related metastability in disordered silicon. 2004 , 93, 215504		5
1348	Adatom ascending at step edges and faceting on fcc metal (110) surfaces. 2004 , 92, 106102		49
1347	Structure and mobility of defects formed from collision cascades in MgO. 2004 , 92, 115505		90
1346	Interaction of neutral vacancies and interstitials with the Si(001) surface. <i>Physical Review B</i> , 2004 , 70,	3-3	10
1345	Effect of Zn on the cation vacancy/electronic oxygen pair in Cd _{1-x} Zn _x Te crystals. <i>Physical Review B</i> , 2004 , 70,	3-3	2

1344	Stable fcc cage of III-IV mixed clusters with large energy gaps: Predictions based on ab initio molecular dynamics simulations. <i>Physical Review B</i> , 2004 , 70,	3-3	5
1343	Computational study of electron states in Au chains on NiAl(110). <i>Physical Review B</i> , 2004 , 70,	3-3	22
1342	Crystal structure and properties of YSiO ₂ N. <i>Physical Review B</i> , 2004 , 69,	3-3	15
1341	Magnetic structure of free iron clusters compared to iron crystal surfaces. <i>Physical Review B</i> , 2004 , 70,	3-3	55
1340	Energetics of Sr adatom interactions on the Mo(112) surface. <i>Physical Review B</i> , 2004 , 69,	3-3	22
1339	First principles study of oxygen vacancy migration in tantalum pentoxide. 2004 , 95, 954-957		26
1338	Atomic scale study of superlow friction between hydrogenated diamond surfaces. <i>Physical Review B</i> , 2004 , 70,	3-3	70
1337	First-principles study of noncommutative band offsets at Ti ₂ O ₃ /Fe ₂ O ₃ (0001) interfaces. <i>Physical Review B</i> , 2004 , 69,	3-3	32
1336	Pressure-driven confinement of hydrogen molecules between graphene sheets in the regime of van der Waals repulsion. <i>Physical Review B</i> , 2004 , 69,	3-3	14
1335	Initial stages of Ge and Si growth near SB monoatomic steps on Si(100). <i>Physical Review B</i> , 2004 , 70,	3-3	3
1334	Density functional theory study of H and H ₂ interacting with NiAl(110). 2004 , 121, 751-60		44
1333	First-principles calculations for the adsorption of water molecules on the Cu(100) surface. <i>Physical Review B</i> , 2004 , 70,	3-3	36
1332	Electronic structure, magnetism, and optical properties of Fe ₂ SiO ₄ fayalite at ambient and high pressures: A GGA+U study. <i>Physical Review B</i> , 2004 , 69,	3-3	43
1331	Nonmetallic nature of In-induced nanoclusters on Si(100). <i>Physical Review B</i> , 2004 , 70,	3-3	8
1330	Metastability of an immiscible Cu-Mo system calculated from first-principles and a derived n-body potential. <i>Physical Review B</i> , 2004 , 69,	3-3	14
1329	Effects of next-nearest-neighbor interactions on the orientation dependence of step stiffness: Reconciling theory with experiment for Cu(001). <i>Physical Review B</i> , 2004 , 70,	3-3	28
1328	Atomistic modeling and thermodynamic interpretation of the bridging phenomenon observed in the Co-Au system. <i>Physical Review B</i> , 2004 , 70,	3-3	7
1327	Epitaxial growth of the diluted magnetic semiconductors Cr _y Ge _{1-y} and Cr _y MnxGe _{1-y} . 2004 , 84, 1725-1727		27

1326	Elastic anomaly for SrTiO ₃ thin films grown on Si(001). <i>Physical Review B</i> , 2004 , 70,	3-3	33
1325	Sulfur point defects in crystalline and amorphous silicon. <i>Physical Review B</i> , 2004 , 70,	3-3	42
1324	Electronic states of linear Au clusters supported on metal surfaces: why are they like those of a particle in a box?. 2004 , 120, 7738-40		9
1323	Oxygen adsorption on Cu(100): First-principles pseudopotential calculations. <i>Physical Review B</i> , 2004 , 70,	3-3	51
1322	Calculation of phonon spectra to predict the high-pressure metastable phase in an equilibrium immiscible Cu ₃ Al system. 2004 , 85, 1517-1519		6
1321	Contrast reversal and shape changes of atomic adsorbates measured with scanning tunneling microscopy. 2004 , 92, 206101		58
1320	Complexity of small silicon self-interstitial defects. 2004 , 92, 045501		60
1319	Theory of Mn supersaturation in Si and Ge. <i>Physical Review B</i> , 2004 , 70,	3-3	34
1318	Theoretical study of the formation, evolution, and breaking of gold nanowires. <i>Physical Review B</i> , 2004 , 69,	3-3	101
1317	Reliable first-principles alloy thermodynamics via truncated cluster expansions. 2004 , 92, 255702		99
1316	Density-functional perturbational theory for dielectric tensors in the ultrasoft pseudopotential scheme. <i>Physical Review B</i> , 2004 , 69,	3-3	22
1315	Electronic structure and bonding in the Y-Si-O-N quaternary crystals. <i>Physical Review B</i> , 2004 , 70,	3-3	32
1314	Role of spin-orbit splitting and dynamical fluctuations in the Si(557)-Au surface. 2004 , 93, 146803		86
1313	Molecular adsorption on the surface of strongly correlated transition-metal oxides: A case study for CO/NiO(100). <i>Physical Review B</i> , 2004 , 69,	3-3	195
1312	Initial growth of Ba on Si(001). <i>Physical Review B</i> , 2004 , 69,	3-3	12
1311	Ab initio calculations to model anomalous fluorine behavior. 2004 , 93, 245901		39
1310	Quantum interference patterns and electron confinement on a two-dimensional metal: A scanning tunneling microscopy study. <i>Physical Review B</i> , 2004 , 69,	3-3	13
1309	Induced Ge spin polarization at the Fe ₂ C interface. <i>Physical Review B</i> , 2004 , 70,	3-3	18

1308	Quantum molecular dynamics simulations of shocked nitrogen oxide. <i>Physical Review B</i> , 2004 , 69,	3-3	14
1307	The effect of Cr doping on Li ion diffusion in LiFePO ₄ from first principles investigations and Monte Carlo simulations. 2004 , 16, 2265-2272		68
1306	Local modes of Fe and Co atoms in NiAl intermetallics. <i>Physical Review B</i> , 2004 , 70,	3-3	17
1305	Dipole moment of a Pb-O vacancy pair in PbTiO ₃ . <i>Physical Review B</i> , 2004 , 69,	3-3	58
1304	Optical phonon softening in strained SrTiO ₃ thin film: First-principles study. 2004 , 85, 5649-5651		9
1303	Evidence from first principles calculations for a bent CO ₂ intermediate in the oxidation of carbon monoxide on the Cu (110) surface. 2004 , 121, 4339-45		7
1302	Wetting of TiC and TiN by metals. <i>Physical Review B</i> , 2004 , 69,	3-3	85
1301	First-principles calculations of steering forces in epitaxial growth. <i>Physical Review B</i> , 2004 , 69,	3-3	12
1300	Neutral boron-interstitial clusters in crystalline silicon. <i>Physical Review B</i> , 2004 , 69,	3-3	18
1299	Electronic structure and exchange interactions in BaVS ₃ . <i>Physical Review B</i> , 2004 , 70,	3-3	22
1298	Structural stability and magnetic properties of metastable Fe-Cu alloys studied by ab initio calculations and molecular dynamics simulations. <i>Physical Review B</i> , 2004 , 69,	3-3	15
1297	Thermodynamics from ab initio computations. <i>Physical Review B</i> , 2004 , 70,	3-3	46
1296	First-principles calculation of the structure and magnetic phases of hematite. <i>Physical Review B</i> , 2004 , 69,	3-3	356
1295	Dynamics of oxygen species on reduced TiO ₂ (110) rutile. <i>Physical Review B</i> , 2004 , 70,	3-3	57
1294	Inversion domain boundaries in ZnO: First-principles total-energy calculations. <i>Physical Review B</i> , 2004 , 69,	3-3	33
1293	Phonon spectrum and soft-mode behavior of MgCNi ₃ . <i>Physical Review B</i> , 2004 , 69,	3-3	33
1292	Impact on electronic correlations on the structural stability, magnetism, and voltage of LiCoPO ₄ battery. <i>Physical Review B</i> , 2004 , 69,	3-3	57
1291	Site selectivity in chemisorption of C on Pd(211). <i>Physical Review B</i> , 2004 , 70,	3-3	16

1290	Theoretical study of Ga-based nanowires and the interaction of Ga with single-wall carbon nanotubes. <i>Physical Review B</i> , 2004 , 70,	3-3	10
1289	SrTiO ₃ /Bi(001) epitaxial interface: A density functional theory study. <i>Physical Review B</i> , 2004 , 70,	3-3	28
1288	Periodic density functional theory study of the crystal morphology of FeZn ₁₃ . <i>Physical Review B</i> , 2004 , 70,	3-3	7
1287	Correlation of magnetic moment versus spacing distance of metastable fcc structured iron. 2004 , 84, 3627-3629		43
1286	Bi _{1-x} Sb _x under high pressure: Effect of alloying on the incommensurate Bi-III type composite structure. <i>Physical Review B</i> , 2004 , 69,	3-3	18
1285	Influence of interfacial texture on solid-state amorphization and associated asymmetric growth in immiscible Cu-Ta multilayers. <i>Physical Review B</i> , 2004 , 70,	3-3	6
1284	Resistivity of hydrogen-loaded Fe/V and Mo/V (100) superlattices: The role of vanadium expansion. <i>Physical Review B</i> , 2004 , 69,	3-3	11
1283	Calculations of electronic structure of Ge ₄₄ Mn ₂ Ba ₈ and Ge ₄₂ Mn ₄ Ba ₈ clathrates. <i>Physical Review B</i> , 2004 , 70,	3-3	5
1282	Defect structure of Ga _{1-x} Mn _x As: A cross-sectional scanning tunneling microscopy study. <i>Physical Review B</i> , 2004 , 70,	3-3	18
1281	Spin driving reconstructions on the GaAs(001):Mn surface. <i>Physical Review B</i> , 2004 , 69,	3-3	16
1280	Ab initio calculations of zinc-blende CrAs/GaAs superlattices. 2004 , 95, 6518-6520		24
1279	First-principles study of adsorption of methanethiol on Co(0001). <i>Physical Review B</i> , 2004 , 70,	3-3	19
1278	Density-functional theory calculations of the adsorption of Cl at perfect and defective Ag(111) surfaces. <i>Physical Review B</i> , 2004 , 69,	3-3	23
1277	A first principles study on the solvation and structure of SO ₄ ²⁻ -(H ₂ O) _n , n=6-12. 2004 , 121, 8299-306		49
1276	Origin of vacancy and interstitial stabilization at the amorphous-crystalline Si interface. 2004 , 96, 3334-3338		6
1275	The influence of bond flexibility and molecular size on the chemically selective bonding of In ₂ O and Ga ₂ O on GaAs(001)-c(2 x 8)/(2 x 4). 2004 , 120, 5745-54		16
1274	Low coverage spontaneous etching and hyperthermal desorption of aluminum chlorides from Cl ₂ /Al(111). 2004 , 121, 9018-30		4
1273	The nonmetallicity of molybdenum clusters. 2004 , 121, 7717-24		42

1272	Interaction between interstitials and arsenic-vacancy complexes in crystalline silicon. 2004 , 85, 4935-4937	13
1271	Low work function of the (1000) Ca ₂ N surface. 2004 , 96, 1751-1753	17
1270	Migration energy for impurity diffusion in crystalline solids: A closer look. 2004 , 96, 7095-7107	8
1269	Transformation strain by chemical disordering in silicon carbide. 2004 , 95, 6466-6469	10
1268	Structural Stability and Optical Properties of hexagonal and cubic CdSe Nanocrystals synthesized in MgO. 2004 , 848, 435	
1267	Hydration and mobility of HO ⁻ (aq). 2004 , 101, 7229-33	140
1266	Ab Initio Study of Magnetic Properties of SiC-Based Diluted Magnetic Semiconductors. 2004 , 264-268, 1237-1240	9
1265	Density-of-states of crystalline 2,2'-bithiophene: ab initio analysis and comparison with inelastic neutron scattering response. 2004 , 16, 7385-7396	15
1264	Indium in silicon: interactions with native defects and with C impurities. 2004 , 810, 311	
1263	The computational design of zinc-blende half-metals and their nanostructures. 2004 , 16, S5525-S5531	13
1262	Theory for the Potential Shift for OH ^{ads} Formation on the Pt Skin on Pt ₃ Cr(111) in Acid. 2004 , 151, E85	52
1261	B2 Phases and their Defect Structures: Part I. Ab Initio Enthalpy of Formation and Enthalpy of Mixing in the Al-Ni-Pt-Ru System. 2004 , 842, 239	
1260	Assessment of the HfN _x , ZrN _x and TiN _x phase diagrams at high pressures and temperatures: balancing between MN and M ₃ N ₄ (M = Hf, Zr, Ti). 2004 , 16, S1235-S1244	38
1259	Behavior of Si Interstitials and Boron-Interstitial Pairs at the Si/SiO ₂ Interface. 2004 , 810, 398	
1258	Atomic structures of nonequilibrium alloys in an immiscible Co ₂ Ag system. 2004 , 19, 1364-1368	9
1257	First-principles design of ferromagnetic nanostructures based on group-IV semiconductors. 2004 , 16, S5735-S5738	7
1256	Electrode Potential-Dependent Stages in OH ^{ads} Formation on the Pt ₃ Cr Alloy (111) Surface. 2004 , 151, E340	33
1255	Structure and stability of possible new alanates. 2004 , 67, 607-613	39

1254	Ab initio molecular-dynamics studies on $\text{Li}_x\text{Mn}_2\text{O}_4$ as cathode material for lithium secondary batteries. 2004 , 67, 28-34		53
1253	Ab-initio electron transport calculations of carbon based string structures. 2004 , 93, 136404		145
1252	Analysis of shear deformations in Al and Cu: empirical potentials versus density functional theory. 2004 , 12, 1017-1029		35
1251	DISSOCIATED WATER ON Si(100): RELATION BETWEEN STM TOPOGRAPH AND ACTUAL GEOMETRY. 2004 , 11, 185-190		3
1250	First-principles calculations of the stability and local structure of β -sialon ceramics on the line $\text{Si}_3\text{N}_4\text{-Ca}_3\text{N}_2\text{:3AlN}$. 2004 , 16, 2931-2939		7
1249	First-principles calculations of the atomistic behaviors in Ni/Al [001] and Al/Ni [001] system. 2004 ,		
1248	Tailoring ferromagnetic chalcopyrites. 2004 , 3, 410-4		139
1247	Density and thermodynamics of hydrogen adsorbed inside narrow carbon nanotubes. 2004 , 46, 584-589		4
1246	Structural relationships, phase stability and bonding of compounds PdS_n ($n=2, 3, 4$). 2004 , 6, 147-155		90
1245	First principles search of hard materials within the Si?C?N ternary system. 2004 , 6, 315-323		16
1244	Energetics of native point defects in cubic silicon carbide. 2004 , 38, 437-444		20
1243	Theory of polaron bandwidth narrowing in organic molecular crystals. <i>Physical Review B</i> , 2004 , 69,	3-3	229
1242	Ab initio theory of charge-carrier conduction in ultrapure organic crystals. 2004 , 85, 1535-1537		163
1241	Spin splitting of s and p states in single atoms and magnetic coupling in dimers on a surface. 2004 , 92, 186802		46
1240	Ab initio study of incorporation of O_2 molecules into Si(001) surfaces: Oxidation by Si ejection. <i>Physical Review B</i> , 2004 , 70,	3-3	22
1239	Initial stages of Mn adsorption on Ge(111). <i>Physical Review B</i> , 2004 , 70,	3-3	52
1238	Hydrogen in aluminum: First-principles calculations of structure and thermodynamics. <i>Physical Review B</i> , 2004 , 69,	3-3	266
1237	First principles analysis of the stability and diffusion of oxygen vacancies in metal oxides. 2004 , 93, 225502		144

1236	Crystal structure and thermodynamic stability of the lithium alanates LiAlH ₄ and Li ₃ AlH ₆ . <i>Physical Review B</i> , 2004 , 69,	3,3	100
1235	Chiral single-wall gold nanotubes. 2004 , 93, 196807		84
1234	Theoretical study of the single-walled gold (5,3) nanotube. 2004 , 85, 2923-2925		32
1233	A comparative theoretical study of Au, Ag and Cu adsorption on TiO ₂ (110) rutile surfaces. 2004 , 21, 537-547		17
1232	The simple cubic structure of Ir clusters and the element effect on cluster structures. 2004 , 383, 67-71		66
1231	Competitive CN and N ₂ formation on Rh(1 1 1): a case of entropic stabilization. 2004 , 385, 52-54		15
1230	Adsorption sites of maleic anhydride on Si(100) revisited: inter- versus intra-row attachment. 2004 , 385, 341-344		4
1229	Potential new candidates for hard materials within the ternary XC ₃ N ₃ (X = B, Al, Ga) stoichiometry. 2004 , 7, 529-535		5
1228	Estimation of exchange current density for ferric/ferrous reaction at electrode surfaces--influence of ionic desolvation and dipolar adsorption. 2004 , 273, 247-55		5
1227	Electronic Structure and Excited-state Properties of Perovskite-like Oxides. 2004 , 268, 554-559		29
1226	Modeling of high-pressure CO dissociation on Pt(1 0 0) and Pt(1 1 1). 2004 , 89, 357-362		5
1225	From first principles to catalytic performance: tracking molecular transformations. 2004 , 59, 4703-4714		54
1224	Theoretical study of segregation of Zn and Pd in Pd _{1-x} Zn _x alloys. 2004 , 548, 291-300		50
1223	FS ⁺ and FS ⁺ (OH) ⁻ defect centers at the MgO(100) surface: cluster and periodic calculations. 2004 , 549, 294-304		24
1222	A combined density functional theory and interatomic potential-based simulation study of the hydration of nano-particulate silicate surfaces. 2004 , 554, 193-210		56
1221	Modeling of the carbon-rich c(4×4) reconstruction on Si(100). 2004 , 554, 90-102		5
1220	Structure and bonding mechanism of cyanide adsorbed on Pt(1 1 1). 2004 , 558, 111-121		30
1219	A DFT investigation of the adsorption of methyl on Rh(111). 2004 , 558, 15-22		20

1218	Atomic and electronic structure of the Si(0 0 1) 2×1 surface. 2004 , 561, 215-226	6
1217	Effect of the electronic structure on CO oxidation on Pd doped Ag(111). 2004 , 566-568, 1063-1066	8
1216	An off-lattice model for Br electrodeposition on Au(1 0 0): from DFT to experiment. 2004 , 563, 169-182	17
1215	Pt thin films on stepped SrTiO ₃ surfaces: SrTiO ₃ (620) and SrTiO ₃ (622). 2004 , 216, 233-245	10
1214	High-pressure phases of MgSiN ₂ from first-principles calculations. 2004 , 78, 717-719	11
1213	Experimental and theoretical evidence for carbon-vacancy binding in austenite. 2004 , 35, 2239-2245	24
1212	Concentrations of native and gold defects in HgCdTe from first principles calculations. 2004 , 33, 737-741	9
1211	Interplay of Electronic Structure and Bulk Properties in 2D and 3D Ternary Carbonitrides from First Principles. 2004 , 630, 2587-2598	6
1210	High-pressure polymorphism in phosphorus nitrides. 2004 , 241, 2319-2325	12
1209	Surface chemistry effects on vacancy and interstitial annihilation on Si(001). 2004 , 241, 2303-2312	6
1208	Valence and conduction band offsets of a ZrO ₂ /SiO _x Ny/n-Si CMOS gate stack: A combined photoemission and inverse photoemission study. 2004 , 241, 2246-2252	52
1207	Pressure-induced phase transition in ErH ₃ . 2004 , 241, 3219-3223	12
1206	Possibility of superconductivity in intercalation compound related to MgB ₂ . 2004 , 96, 457-462	5
1205	The vibrational spectrum of magnesium hydride from inelastic neutron scattering and density functional theory. 2004 , 108, 38-41	35
1204	Reactivity of Pd doped Ag surfaces. 2004 , 74, 169-172	1
1203	Restoring the band gap of metal oxide surfaces by redox adsorption. 2004 , 709, 87-96	4
1202	CO oxidation over anatase TiO ₂ -(001). 2004 , 709, 73-78	47
1201	Atomistic simulations of Cu deposition on the α -Al ₂ O ₃ (0001) surface. 2004 , 709, 79-85	1

1200	Modeling catalytic reduction of NO by ammonia over V ₂ O ₅ . 2004 , 55, 169-236	71
1199	Revisit to the Ising model for order-disorder phase transition on Si(001). 2004 , 554, 150-158	5
1198	Assessment of heterochiral and homochiral glycine adlayers on Cu(1 1 0) using density functional theory. 2004 , 548, 301-308	97
1197	Multilayer relaxations of (311), (331) and (210) fcc transition metal surfaces studied by pseudopotential DFT calculations. 2004 , 548, 309-316	17
1196	Comparative DFT study of the adsorption of 1,3-butadiene, 1-butene and 2-cis/trans-butenes on the Pt(111) and Pd(111) surfaces. 2004 , 549, 121-133	80
1195	Conveying chirality onto the electronic structure of achiral metals: (R,R)-tartaric acid on nickel. 2004 , 554, 141-149	46
1194	Effect of relaxation on structure and reactivity of anatase (1 0 0) and (0 0 1) surfaces. 2004 , 552, 169-179	69
1193	Sum frequency generation and density functional studies of CO _H interaction and hydrogen bulk dissolution on Pd(111). 2004 , 554, 43-59	64
1192	Mechanisms of monovacancy annihilation and type-A defect creation on Si(0 0 1) $\sqrt{3} \times \sqrt{3}$. 2004 , 555, 187-192	6
1191	Dissociative adsorption of N ₂ on the W(1 0 0) surface. 2004 , 556, 129-144	37
1190	New structural model of the high-index Si(5512)2 $\sqrt{3} \times \sqrt{3}$ surface. 2004 , 557, 183-189	33
1189	On the geometric structure of the (0 0 0 1) hematite surface. 2004 , 558, 4-14	46
1188	Adsorption of Mn atoms on the Si(1 0 0) surface. 2004 , 566-568, 688-692	9
1187	DFT study of Cl/MgO(1 0 0), influence of the stoichiometry. 2004 , 566-568, 693-697	15
1186	DFT plane-wave calculations of the Rh/MgO(0 0 1) interface. 2004 , 566-568, 977-982	9
1185	S and O adsorption on pure and Ge doped Ag(111). 2004 , 566-568, 1067-1070	1
1184	Water molecule dissociation at ice/MgO(1 0 0) interface. 2004 , 562, 237-246	8
1183	Critical layer thickness in Stranski-Krastanow growth of Ge on Si(001). 2004 , 562, L225-L230	15

1182	TiO ₂ -rich reconstructions of SrTiO ₃ (0 0 1): a theoretical study of structural patterns. 2004 , 573, 446-456	54
1181	Mn-doped ZnSnAs ₂ chalcopyrites: an ab initio study of antiferromagnetic semiconductors. 2004 , 272-276, E243-E244	9
1180	Conductance of Ni nanocontacts within first-principle approach. 2004 , 272-276, 1730-1731	8
1179	Electronic structure and magnetism of diluted magnetic semiconductors and derivatives. 2004 , 272-276, E1581-E1582	
1178	Final state effects in the X-ray absorption spectra of La _{0.7} Sr _{0.3} MnO ₃ . 2004 , 272-276, 1780-1781	
1177	Electronic structure and magnetic moments of 3d transition metal-doped ZnO. 2004 , 282, 275-278	106
1176	Defect energetics of β -SiC using a new tight-binding molecular dynamics model. 2004 , 329-333, 1219-1222	18
1175	Molecular dynamics simulation of displacement cascades in FeCr alloys. 2004 , 329-333, 1156-1160	63
1174	Simulation of radiation damage in Fe alloys: an object kinetic Monte Carlo approach. 2004 , 335, 121-145	243
1173	High potential positive materials for lithium-ion batteries: transition metal phosphates. 2004 , 65, 229-233	77
1172	Cyanide adsorption on gold electrodes: a combined surface enhanced Raman spectroscopy and density functional theory study. 2004 , 563, 111-120	49
1171	Elastic properties of platinum Rh and Rh ₃ X compounds. 2004 , 331, 400-403	48
1170	Atomic-scale ab initio study of the ZrH system: II. Interaction of H with plane defects and mechanical properties. 2004 , 52, 1495-1502	74
1169	Effects of cobalt intergranular segregation on interface energetics in WC-Co. 2004 , 52, 2199-2207	77
1168	A combined CALPHAD/first-principles remodeling of the thermodynamics of AlBr: unsuspected ground state energies by bounding up the (un)usual suspects. 2004 , 52, 2739-2754	63
1167	First principles simulations of Cu and Au deposition on β -Al ₂ O ₃ (0 0 0 1) surface. 2004 , 238, 228-232	18
1166	Atomic geometry and theoretical scanning tunneling microscopy images of K chains on InAs(110). 2004 , 237, 200-205	
1165	Two-dimensional arrangement of CH ₃ NH ₂ adsorption on Si(0 0 1)-2 \times 1. 2004 , 385, 144-148	8

1164	Ab initio study of CNT NO ₂ gas sensor. 2004 , 387, 271-276	388
1163	What the stretch frequency spectrum of D ₂ O/Ru(0001) does and does not mean. 2004 , 389, 92-95	26
1162	Intermolecular transfer integrals for organic molecular materials: can basis set convergence be achieved?. 2004 , 390, 110-115	128
1161	Modeling of FS ₂ ⁺ center at the magnesium oxide (1 0 0) hydrated surface. 2004 , 391, 120-123	3
1160	From planar to three-dimensional structural transition in gold clusters and the spin-orbit coupling effect. 2004 , 392, 452-455	167
1159	Surface energetics of hydroxyapatite: a DFT study. 2004 , 396, 38-42	50
1158	Strong and weak adsorption of CO on CeO ₂ surfaces from first principles calculations. 2004 , 396, 384-392	95
1157	The role of surface elasticity in giant corrugations observed by scanning tunneling microscopes. 2004 , 397, 354-359	26
1156	A reexamination of the chemisorption and desorption of ozone on the exterior of a (5,5) single-walled carbon nanotube. 2004 , 398, 297-303	61
1155	Electronic structures of InTaO ₄ , a promising photocatalyst. 2004 , 398, 449-452	35
1154	Theoretical study of propene adsorbed on sulphated Pt(111). 2004 , 399, 295-299	4
1153	Electron-count control on adsorption upon reducible and irreducible clean metal-oxide surfaces. 2004 , 89, 269-278	49
1152	Electronic structure of the extended vanadyl pyrophosphate (1 0 0) surface. 2004 , 91-92, 177-180	6
1151	Adsorption of Pd atoms on γ -Al ₂ O ₃ : a density functional study of metal-support interactions. 2004 , 238, 82-85	20
1150	Elastic polarizable environment cluster embedding approach for water adsorption on the γ -Al ₂ O ₃ (0001) surface. A density functional study. 2004 , 6, 4505-4513	16
1149	Rh and Pt nanoparticles supported by CeO ₂ : Metal-support interaction upon high-temperature reduction observed by electron microscopy. 2004 , 6, 5244-5249	34
1148	Density functional study of methoxide decomposition on PdZn(100). 2004 , 6, 4499-4504	28
1147	Effects of Ag and Ni Additives on Zn Diffusion in Steel Hot-Dip Galvanizing: An ab Initio Molecular Dynamics Simulation. 2004 , 16, 5567-5573	7

1146	Effects of metal buffer layer on the morphology of the ZnO columns. 2004,		
1145	Inner shell definition and absolute hydration free energy of K+(aq) on the basis of quasi-chemical theory and ab initio molecular dynamics. 2004, 6, 1966-1969		77
1144	Collective ionic motion in oxide fast-ion-conductors. 2004, 6, 3052-3055		23
1143	Optical Spectra, Properties and First Principles Computations of Ba(Fe, Nb)O ₃ and Pb(Fe, Nb)O ₃ . 2004, 302, 279-283		10
1142	Detection and visualization of anomalous structures in molecular dynamics simulation data.		10
1141	Mechanisms for the reconstructive phase transition between the B1 and B2 structure types in NaCl and PbS. <i>Physical Review B</i> , 2004, 69,	3-3	32
1140	Nitrogen doping and chirality of carbon nanotubes. <i>Physical Review B</i> , 2004, 70,	3-3	96
1139	Two-dimensional hydration shells of alkali metal ions at a hydrophobic surface. 2004, 121, 12572-6		21
1138	Electronic structure and dielectric properties of dielectric gate material (ZrO ₂) _x (SiO ₂) _{1-x} . 2004, 95, 7918-7924		19
1137	Phase stability of nanocarbon in one dimension: nanotubes versus diamond nanowires. 2004, 120, 3817-21		49
1136	First principles study of transition-metal substitutions in SmCo permanent magnets. 2004, 85, 2286-2288		27
1135	Evidence for interstitial hydrogen as the dominant electronic defect in nanometer alumina films. <i>Physical Review B</i> , 2004, 69,	3-3	44
1134	Density Functional Theory Study of Silica Zeolite Structures: Stabilities and Mechanical Properties of SOD, LTA, CHA, MOR, and MFI. 2004, 108, 9208-9215		79
1133	Electron-deficient bonding in rhomboid rings. 2004, 126, 13119-31		39
1132	Flanged nanotube-electrode junctions. 2004, 15, 1226-1232		5
1131	Oxygen vacancies on TiO ₂ (110) from first principles calculations. 2004, 121, 7427-33		67
1130	Proposed Definition of Microchemical Inhomogeneity and Application To Characterize Some Selected Miscible/Immiscible Binary Metal Systems. 2004, 108, 16071-16076		20
1129	Reduced SnO ₂ surfaces by first-principles calculations. 2004, 84, 909-911		85

1128	Nature of one-dimensional short hydrogen bonding: bond distances, bond energies, and solvent effects. 2004 , 126, 2186-93		75
1127	Distribution of Cations in FeSbO ₄ : A Computer Modeling Study. 2004 , 16, 1954-1960		33
1126	Effect of strain on atomic ordering and action of surfactants in ternary alloy thin films. <i>Physical Review B</i> , 2004 , 70,	3-3	4
1125	Theoretical study of bulk and surface oxygen and aluminum vacancies in α -Al ₂ O ₃ . <i>Physical Review B</i> , 2004 , 69,	3-3	74
1124	Reactivity of the Oxygen Sites in the V ₂ O ₅ /TiO ₂ Anatase Catalyst. 2004 , 108, 15679-15685		37
1123	Energetics and electronic structure of stacking faults in ZnO. <i>Physical Review B</i> , 2004 , 70,	3-3	82
1122	Density-functional band-structure calculations for La-, Y-, and Sc-filled CoP ₃ -based skutterudite structures. <i>Physical Review B</i> , 2004 , 70,	3-3	26
1121	Design of Potential Hydrogen-Storage Materials Using First-Principle Density-Functional Calculations. 2004 , 4, 471-477		50
1120	Structural and electronic properties of oxygen vacancies in cubic and antiferrodistortive phases of SrTiO ₃ . <i>Physical Review B</i> , 2004 , 69,	3-3	90
1119	The Simple Cubic Structure of Ruthenium Clusters. 2004 , 108, 2140-2147		63
1118	CH ₃ O decomposition on PdZn(111), Pd(111), and Cu(111). A theoretical study. 2004 , 20, 8068-77		125
1117	Vibrational behavior of adsorbed CO ₂ on single-walled carbon nanotubes. 2004 , 120, 5377-86		68
1116	Ice tessellation on a hydroxylated silica surface. 2004 , 92, 146102		79
1115	Impurity-doped Si ₁₀ cluster: Understanding the structural and electronic properties from first-principles calculations. <i>Physical Review B</i> , 2004 , 70,	3-3	41
1114	Atomic and Electronic Structure of Pyridine on Ge(100). 2004 , 108, 15229-15232		30
1113	Scanning Tunneling Microscopy and Theoretical Study of Competitive Reactions in the Dissociative Chemisorption of CCl ₄ on Iron Oxide Surfaces. 2004 , 108, 16753-16760		19
1112	Trends in the Chemisorption of Aromatic Molecules on a Pt(111) Surface: Benzene, Naphthalene, and Anthracene from First Principles Calculations. 2004 , 108, 12084-12091		97
1111	Chains of gold atoms with tailored electronic states. <i>Physical Review B</i> , 2004 , 69,	3-3	237

1110	Experimental determination of valence band maxima for SrTiO ₃ , TiO ₂ , and SrO and the associated valence band offsets with Si(001). 2004 , 22, 2205	240
1109	Vibrational Analysis of the Inelastic Neutron Scattering Spectrum of Tetramethylammonium Borohydride by Molecular Dynamics Simulations and Electronic Structure Calculations. 2004 , 108, 11369-11374 ¹⁰	
1108	Dielectric Permittivity Study of KTaO ₃ Weakly Doped by 6Li Isotope. 2004 , 302, 203-206	1
1107	Phase stability in the systems AeAl(2-x)Mgx (Ae = Ca, Sr, Ba): electron concentration and size controlled variations on the laves phase structural theme. 2004 , 43, 4751-60	25
1106	Density Functional Theory Study of Co, Rh, and Ir Atoms Deposited on the $\bar{1}11$ -Al ₂ O ₃ (0001) Surface. 2004 , 108, 15671-15678	29
1105	Ethylene Decomposition on Rh(100): Theory and Experiment \square 2004 , 108, 14541-14548	22
1104	Formation of Schottky Defects at the Surface of MgO, TiO ₂ , and SnO ₂ : A Comparative Density Functional Theoretical Study. 2004 , 108, 12858-12864	37
1103	Structural and Spectroelectrochemical Study of Carbonate and Bicarbonate Adsorbed on Pt(111) and Pd/Pt(111) Electrodes. 2004 , 108, 17928-17939	37
1102	Effects of Subsurface Boron and Phosphorus on Surface Reactivity of Si(001): Water and Ammonia Adsorption. 2004 , 108, 16147-16153	3
1101	Theoretical Studies of N ₂ O Adsorption and Reactivity to N ₂ and NO on Rh(111). 2004 , 108, 17921-17927	33
1100	Adsorption of Cyclopentene on Pt(111) and Ordered PtnSn/Pt(111) Surface Alloys. 2004 , 108, 18960-18971	24
1099	Ab initio Investigation of the Early Stage of Nano-scale Thin Film Growth: Al and Co Adatoms on Co (111) Surface. 2004 , 43, 3815-3817	4
1098	Density-functional theory of xanthate adsorption on the pyrite FeS ₂ (100) surface. 2004 , 84, 175-182	13
1097	Molecular Simulations of Anhydrous Na ₆ [Al ₆ Si ₆ O ₂₄] Sodalite. 2004 , 16, 2121-2133	26
1096	Chemisorption of Benzene on Pt(111), Pd(111), and Rh(111) Metal Surfaces: A Structural and Vibrational Comparison from First Principles. 2004 , 108, 5653-5665	140
1095	Huge magneto-optical effects in half-metallic double perovskites. <i>Physical Review B</i> , 2004 , 70,	3-3 19
1094	Nucleation kinetics during homoepitaxial growth of TiN(001) by reactive magnetron sputtering. <i>Physical Review B</i> , 2004 , 70,	3-3 43
1093	The properties of methylene- and amine-substituted zeolites from first principles. 2004 , 126, 1843-8	53

1092	A note on temperature-dependent band narrowing in oligo-acene crystals. 2004 , 16, 2023-2032		16
1091	Redox-Induced Structural Change in Anode Materials Based on Tetrahedral (MPn4)x- Transition Metal Pnictides. 2004 , 16, 1002-1013		57
1090	Planar tetracoordinate carbon in extended systems. 2004 , 126, 15309-15		113
1089	Coverage Dependent Adsorption of Acrolein on Pt(111) from a Combination of First Principle Theory and HREELS Study. 2004 , 108, 9085-9093		68
1088	Effect of electron correlations on the electronic and magnetic structure of Ti-doped α -hematite. <i>Physical Review B</i> , 2004 , 69,	3-3	62
1087	Ab-initio high-pressure alloying of iron and potassium: Implications for the Earth's core. 2004 , 31, n/a-n/a		25
1086	The location of adsorbed hydrogen in graphite nanostructures. 2004 , 126, 13095-9		41
1085	Theoretical study of crossed and parallel carbon nanotube junctions and three-dimensional grid structures. <i>Physical Review B</i> , 2004 , 70,	3-3	33
1084	Theoretical Interpretation of the IR Spectrum of Propyne on Cu(111). 2004 , 108, 18297-18305		20
1083	Ab initio study of the (0001) surfaces of hematite and chromia: Influence of strong electronic correlations. <i>Physical Review B</i> , 2004 , 70,	3-3	313
1082	Binding of propene on small gold clusters and on Au(111): simple rules for binding sites and relative binding energies. 2004 , 121, 3756-66		90
1081	Interstitial oxygen in Si and Si _{1-x} Ge _x . <i>Physical Review B</i> , 2004 , 69,	3-3	25
1080	Oxygen neutral defects in silica: Origin of the distribution of the formation energies. 2004 , 66, 680-686		18
1079	Predicting the Energetics, Phase Stability, and Morphology Evolution of Faceted and Spherical Anatase Nanocrystals. 2004 , 108, 18435-18440		106
1078	Energetics and diffusivity of indium-related defects in silicon. <i>Physical Review B</i> , 2004 , 69,	3-3	18
1077	Structures of Platinum Clusters: 'Planar or Spherical?' 2004 , 108, 8605-8614		221
1076	Experimental evidence for a high-pressure isostructural phase transition in osmium. 2004 , 93, 095502		111
1075	Early chemistry in hot and dense nitromethane: molecular dynamics simulations. 2004 , 120, 10146-53		94

1074	Structure and Energetics of LiBH ₄ and Its Surfaces: A First-Principles Study <i>Physical Review B</i> , 2004 , 108, 8682-8690		63
1073	Lattice dynamics in PbMg _{1/3} Nb _{2/3} BO ₃ . <i>Physical Review B</i> , 2004 , 70,	3-3	99
1072	Water adsorption on metal surfaces: A general picture from density functional theory studies. <i>Physical Review B</i> , 2004 , 69,	3-3	404
1071	Ab initio morphology and surface thermodynamics of α -Al ₂ O ₃ . <i>Physical Review B</i> , 2004 , 69,	3-3	102
1070	Density functional study of the adsorption of propene on silver clusters, Ag _m q (m=1-8; q=0, +1). 2004 , 121, 9925-9930		37
1069	Fundamental Properties of SiC: Crystal Structure, Bonding Energy, Band Structure, and Lattice Vibrations. 2004 , 63-87		4
1068	The Nowotny chimney ladder phases: following the c(pseudo) clue toward an explanation of the 14 electron rule. 2004 , 43, 6151-8		70
1067	The Nowotny chimney ladder phases: whence the 14 electron rule?. 2004 , 43, 6159-67		83
1066	Complete Spin Polarization for a Carbon Nanotube with an Adsorbed Atomic Transition-Metal Chain. 2004 , 4, 561-563		73
1065	Ab initio simulations of the electrical and optical properties of shock-compressed SiO ₂ . <i>Physical Review B</i> , 2004 , 70,	3-3	51
1064	Ab initio thermodynamics of oxide surfaces: O ₂ on Fe ₂ O ₃ (0001). <i>Physical Review B</i> , 2004 , 69,	3-3	133
1063	Linear and nonlinear optical properties of carbon nanotubes from first-principles calculations. <i>Physical Review B</i> , 2004 , 69,	3-3	214
1062	First-principles calculation of defect-formation energies in the Y ₂ (Ti,Sn,Zr) ₂ O ₇ pyrochlore. <i>Physical Review B</i> , 2004 , 70,	3-3	123
1061	Transport in proton conductors for fuel-cell applications: simulations, elementary reactions, and phenomenology. 2004 , 104, 4637-78		1744
1060	A computer modelling study of the uptake and segregation of fluoride ions at the hydrated hydroxyapatite (0001) surface: introducing a Ca ₁₀ (PO ₄) ₆ (OH) ₂ potential model. 2004 , 6, 1860-1866		84
1059	Density functional study of the adsorption of propene on mixed gold-silver clusters, Au _n Ag _m : Propensity rules for binding. 2004 , 121, 9931-9937		56
1058	Structural stability and electronic structure for Li ₃ AlH ₆ . <i>Physical Review B</i> , 2004 , 69,	3-3	36
1057	First-principles study of hydrogen diffusion in α -Al ₂ O ₃ and liquid alumina. <i>Physical Review B</i> , 2004 , 69,	3-3	59

1056	From nanodiamond to diamond nanowires: structural properties affected by dimension. 2004 , 84, 899-907		20
1055	Ab initio study of the phase diagram of epitaxial BaTiO ₃ . <i>Physical Review B</i> , 2004 , 69,	3-3	201
1054	Ab initio molecular dynamics simulation of liquid Al _x Ge _{1-x} alloys. <i>Physical Review B</i> , 2004 , 70,	3-3	5
1053	Free energy of adsorption of water and metal ions on the [1014] calcite surface. 2004 , 126, 10152-61		251
1052	Electronic properties of rutile TiO ₂ ultrathin films: Odd-even oscillations with the number of layers. <i>Physical Review B</i> , 2004 , 70,	3-3	136
1051	High-coverage stable structures of potassium adsorbed on single-walled carbon nanotubes. <i>Physical Review B</i> , 2004 , 69,	3-3	16
1050	First principles study of the ferromagnetism in Ga _{1-x} Mn _x As semiconductors. 2004 , 16, 8243-8250		15
1049	The Formation and Stability of Adsorbed Formyl as a Possible Intermediate in Fischer-Tropsch Chemistry on Ruthenium. 2004 , 108, 3614-3624		48
1048	Atomic strings of group IV, III-V, and II-VI elements. 2004 , 85, 6179-6181		29
1047	Comparative study of defect energetics in HfO ₂ and SiO ₂ . 2004 , 84, 1492-1494		102
1046	The structure of alpha-Zn ₄ Sb ₃ : ordering of the phonon-glass thermoelectric material beta-Zn ₄ Sb ₃ . 2004 , 126, 16306-7		129
1045	Ab-initio simulation of (a/2)<110> screw dislocations in TiAl. 2004 , 84, 401-413		44
1044	Density functional study of the adsorption of a C ₆₀ monolayer on Ag(111) and Au(111) surfaces. <i>Physical Review B</i> , 2004 , 69,	3-3	153
1043	Stable geometries and magnetic properties of single-walled carbon nanotubes doped with 3d transition metals: A first-principles study. <i>Physical Review B</i> , 2004 , 69,	3-3	219
1042	Para to ortho transition of metallic dimers on Si(001). <i>Physical Review B</i> , 2004 , 69,	3-3	11
1041	First-principles elastic constants and phonons of Pu. <i>Physical Review B</i> , 2004 , 70,	3-3	30
1040	First-principles study of Li ion diffusion in LiFePO ₄ . <i>Physical Review B</i> , 2004 , 69,	3-3	209
1039	Ab initio Monte Carlo simulations for finite-temperature properties: application to lithium clusters and bulk liquid lithium. 2004 , 29, 145-151		13

1038	Ab initio study on the lattice instability of silicon and aluminum under [0 0 1] tension. 2004 , 29, 397-406	14
1037	Static polarizability of carbon nanotubes: ab initio independent-particle calculations. 2004 , 30, 269-273	41
1036	Chemical-bonding and high-pressure studies on hydrogen-storage materials. 2004 , 30, 349-357	27
1035	Electronic structure of bulk and (001) surface layers of pyrite FeS ₂ . 2004 , 30, 358-363	35
1034	First-principles calculation on free energy of precipitate nucleation. 2004 , 28, 173-176	34
1033	Thermochemistry and crystal structures of lithium, sodium and potassium alanates as determined by ab initio simulations. 2004 , 372, 92-96	37
1032	Electronic structure and Rietveld refinement parameters of Ti-doped sodium alanates. 2004 , 375, 1-10	79
1031	A theoretical search for intermetallic compounds and solution phases in the binary system Sn/Zn. 2004 , 379, 110-116	6
1030	Ti ₂ ZrNi and Ti ₂ HfNi quasicrystals and approximants as hydrogen storage alloys. 2004 , 334-335, 461-465	12
1029	A DFT study of the compressibility of amorphous silicon oxynitride. 2004 , 345-346, 720-723	6
1028	Direct observation of charge transfer at a MgO(111) surface. 2004 , 92, 026101	33
1027	Atomic and electronic structure of the Si(001)2×1 chemisorption system at 0.5 monolayer coverage. <i>Physical Review B</i> , 2004 , 69,	3-3 9
1026	Crystal structure of KAlH ₄ from first principle calculations. 2004 , 363, L8-L12	39
1025	Lattice model for the properties of non-stoichiometric cubic and hexagonal molybdenum nitride. 2004 , 364, 13-16	12
1024	Structural phase transitions in the Cu-based Cu ₃ solid solutions studied by molecular dynamics simulation. 2004 , 366, 205-212	5
1023	Ab Initio Calculations of Intermediates of Oxygen Reduction on Low-Index Platinum Surfaces. 2004 , 151, A2016	160
1022	Sampling the diffusion paths of a neutral vacancy in silicon with quantum mechanical calculations. <i>Physical Review B</i> , 2004 , 70,	3-3 70
1021	Quasiharmonic approach to a second-order phase transition. <i>Physical Review B</i> , 2004 , 70,	3-3 17

1020	Effects of particle morphology and surface hydrogenation on the phase stability of TiO ₂ . <i>Physical Review B</i> , 2004 , 70,	3-3	191
1019	Ab initio calculations of cohesive energies of Fe-based glass-forming alloys. <i>Physical Review B</i> , 2004 , 70,	3-3	70
1018	Ab initio study of foreign interstitial atom (C, N) interactions with intrinsic point defects in β -Fe. <i>Physical Review B</i> , 2004 , 69,	3-3	312
1017	Diamond under pressure: Ab-initio calculations of the equation of state and optical phonon frequency revisited. 2004 , 24, 101-110		15
1016	Modelling, refinement and analysis of the β -type Bi_2O_3 -related superstructure in the Bi_2O_3 - Nb_2O_5 system. 2004 , 177, 1838-1846		52
1015	Polarising Ability of the Metal Surface Atoms of a Catalyst and the Work Function. 2004 , 22, 693-706		1
1014	Structural Stability of the Metastable Solid Solution in the Equilibrium Immiscible Ag-Mo System Predicted by ab Initio Derived Potential. 2004 , 73, 1222-1227		5
1013	Atomistic Modeling of Metastable Phase Selection of a Highly Immiscible Ag-M System. 2004 , 73, 2023-2027		6
1012	Free-Energy Calculation of Precipitate Nucleation in an Fe-Cu-Ni Alloy. 2004 , 45, 1978-1981		28
1011	First Principles Calculation of Free Energy on Precipitate Nucleation. 2004 , 68, 973-976		2
1010	Interaction between Substitutional and Interstitial Elements in α -Fe Studied by First-Principles Calculation. 2004 , 68, 977-982		8
1009	Vibrational Contribution on Nucleation Free Energy of Cu Precipitates in Fe-Cu System. 2004 , 45, 1473-1477		7
1008	Binding Energy and the Heat of Chemisorption on Metallic Catalysts α Thermodynamic Aspect. 2005 , 23, 161-172		1
1007	Structural Stability and Homogeneity of the Nonequilibrium Co-Ag Alloys. 2005 , 74, 375-381		6
1006	Interaction between Substitutional and Interstitial Elements in α iron Studied by First-principles Calculation. 2005 , 46, 1140-1147		11
1005	Confinement of Bloch waves in YSi ₂ nanostructures on Si(111). 2005 , 69, 784-790		4
1004	Reactivity between molybdenum and TiO ₂ (110) surfaces: evidence of a sub-monolayer mode and a multilayer mode. 2005 , 244, 403-407		12
1003	Surface diffusion and incorporation of adatom in Co/Al (0 0 1) system. 2005 , 178, 47-51		6

1002	Order in the disordered state: local structural entities in the fast ion conductor Ba ₂ In ₂ O ₅ . 2005 , 178, 346-355	38
1001	Transition metal intermetallics: Structure maps based on quantum mechanical stability. 2005 , 178, 1269-1283	19
1000	Hydrides with the perovskite structure: General bonding and stability considerations and the new representative CaNiH ₃ . 2005 , 178, 3381-3388	38
999	Ab initio study of phonons in the rutile structure of TiO ₂ . 2005 , 66, 1069-1073	56
998	Modelling polymer-derived ceramics. 2005 , 25, 163-174	39
997	Annealing of vacancy complexes in P-doped silicon. 2005 , 228, 218-225	24
996	Developing pair potentials for simulating radiation damage in complex oxides. 2005 , 228, 288-292	40
995	Structural stabilities and electronic structures of Ti atomic chains. 2005 , 30, 138-142	14
994	First principles study of wurtzite and zinc blende GaN: a comparison of the electronic and optical properties. 2005 , 336, 145-151	26
993	Ab initio investigation of the surface properties of Cu(111) and Li diffusion in Cu thin film. 2005 , 337, 247-255	32
992	The role of the hydrogen bonding network for the shear modulus of PIPD. 2005 , 46, 9144-9154	18
991	Influence of nitrogen stoichiometry on properties of low-compressibility advanced nitrides. 2005 , 358, 72-76	11
990	Orientation of ethoxy, mono-, di-, and tri-fluoroethoxy on Cu(111): a DFT study. 2005 , 228, 77-82	16
989	Theory and experiments on the structure of γ -alumina films grown on Ni ₃ Al. 2005 , 228, 83-87	8
988	First-principles simulations of dislocation cores. 2005 , 400-401, 59-67	49
987	Ab initio study of the effect of hydrogen and point defects on arsenic segregation at Si (100)/SiO ₂ interfaces. 2005 , 124-125, 359-362	
986	RPV steel microstructure evolution under irradiation: a multiscale approach. 2005 , 228, 111-121	17
985	Ab initio calculations of vacancy interactions with solute atoms in bcc Fe. 2005 , 228, 137-141	60

984	Exploring long-time response to radiation damage in MgO. 2005 , 228, 260-273	16
983	Threshold displacement energies in rutile TiO ₂ : A molecular dynamics simulation study. 2005 , 239, 191-201	47
982	Quantum mechanics calculations on the diastereomeric salts of cyclic phosphoric acids with ephedrine. 2005 , 717, 205-214	
981	Theoretical study of hydrated sulfuric acid: clusters and periodic modeling. 2005 , 718, 71-76	20
980	Strain effect on dielectric property of SrTiO ₃ lattice: first-principles study. 2005 , 475, 97-101	8
979	Structural and dielectric properties of crystalline and amorphous ZrO ₂ . 2005 , 486, 125-128	142
978	Effects of oxygen-gas flow rate on lattice dynamics and microstructure for Ga-doped ZnO thin films prepared by reactive plasma deposition. 2005 , 38, 369-376	12
977	Nanocomposites—new material design concept. 2005 , 6, 2-10	145
976	The structure of formate species on Pd(111) calculated by density functional theory and determined using low energy electron diffraction. 2005 , 574, 166-174	48
975	Chemisorption of atomic chlorine on metal surfaces and the interpretation of the induced work function changes. 2005 , 574, 297-305	64
974	Atomic and electronic structure of the Si(001)2×1Li chemisorption system at 1.0 monolayer coverage. 2005 , 574, 233-243	4
973	Oscillatory interaction between O impurities and Al adatoms on Al(111) and its effect on nucleation and growth. 2005 , 575, 89-102	9
972	Cu, Ag and Au atoms deposited on the β -Al ₂ O ₃ (0001) surface: a comparative density functional study. 2005 , 575, 189-196	55
971	Pd nanoclusters at the MgO(1 0 0) surface. 2005 , 575, 197-209	39
970	Dynamical properties and the proton transfer mechanism in the wetting water layer on Pt(111). 2005 , 575, 300-306	32
969	Molecular precursor-mediated methanol dissociation on Si(111)7×7: ab initio study. 2005 , 577, 15-21	5
968	Adsorption and reaction of N ₂ H ₄ on Si(1 0 0)-2 × 1: A computational study with single- and double-dimer cluster models. 2005 , 579, 197-214	7
967	DFT study of Pt adsorption on low index SrTiO ₃ surfaces: SrTiO ₃ (100), SrTiO ₃ (111) and SrTiO ₃ (110). 2005 , 581, 66-87	39

966	Cobalt concentration effect in Pt _{1-x} Cox on the reversible potential for forming OHads from H2Oads in acid solution. 2005 , 581, 105-117	40
965	Surface segregation in palladium based alloys from density-functional calculations. 2005 , 583, 100-106	101
964	Comparison of the reduction of metal oxide surfaces: TiO2-anatase, TiO2-rutile and SnO2-rutile. 2005 , 583, 107-117	91
963	The first-principle study on chlorine-modified silver surfaces. 2005 , 584, 187-198	22
962	Structure and vibrational spectra of crystalline SiO2 ultra-thin films on Mo(1 1 2). 2005 , 584, 225-236	62
961	Phase transition at finite temperature in one dimension: Adsorbate ordering in Ba/Si(111)3 $\sqrt{3}$. 2005 , 585, L171-L176	7
960	Theoretical study of oxygen adsorption at the Fe(110) and (100) surfaces. 2005 , 590, 88-100	123
959	A simple chemical view of relaxations at stoichiometric (1 1 0) surfaces of rutile-structure type oxides: A first-principles study of stishovite, SiO2. 2005 , 594, 70-82	9
958	CO adsorption on monometallic Pd, Rh, Cu and bimetallic PdCu and RhCu monolayers supported on Ru(0001). 2005 , 598, 144-155	31
957	Atomic structure of the 6H β -SiC(0001) nanomesh. 2005 , 596, 176-186	165
956	Evolution of Fermi level position and Schottky barrier height at Ni/MgO(001) interface. 2005 , 599, 255-261	15
955	Effects of hydrogen on electronic properties of doped diamond. 2005 , 43, 1009-1014	15
954	Adsorption of atomic and molecular oxygen on Cu(100). 2005 , 100, 403-406	28
953	Adsorption and decomposition of H2S on Pd(1 1 1) surface: a first-principles study. 2005 , 99, 315-322	81
952	Structure and binding site of acetate on Pd(1 1 1) determined using density functional theory and low energy electron diffraction. 2005 , 105, 74-77	29
951	First principles calculations of the adsorption and diffusion of hydrogen on Fe(100) surface and in the bulk. 2005 , 105, 44-65	74
950	Nucleation and growth of 1B metal clusters on rutile TiO2(1 1 0): Atomic level understanding from first principles studies. 2005 , 105, 78-84	22
949	Predicting yield-stress anomalies in L12 alloys: Ni3Ge β -3Ge pseudo-binaries. 2005 , 53, 3601-3612	22

948	Kinetic Monte Carlo study of AlMg precipitation. 2005 , 53, 3721-3728		19
947	Comparative theoretical study of the structure and bonding of propyne on the Pt(111) and Pd(111) surfaces. 2005 , 309, 33-39		13
946	Probing vibrational excitations in molecular crystals by inelastic scattering: From neutrons to X-rays. 2005 , 317, 153-158		9
945	The role of water in the initial steps of methanol oxidation on Pt(111). 2005 , 319, 185-191		62
944	Lattice modes of hexamethylbenzene studied by inelastic neutron scattering. 2005 , 317, 143-152		8
943	Ground states of potassium adsorbate on single-walled carbon nanotubes. 2005 , 169, 20-23		5
942	Consistent picture for the wetting structure of water/Ru(0001). 2005 , 402, 384-388		54
941	Role of surface geometry and electronic structure in STM images of O/Ru(0001). 2005 , 405, 131-135		20
940	Adsorption thermodynamics of acrolein on Pt (111) in realistic temperature and pressure from first-principle calculations. 2005 , 405, 434-439		26
939	Simulating temperature programmed desorption directly from density functional calculations: How adsorbate configurations relate to desorption features. 2005 , 407, 227-231		9
938	A wetting layer breaks the ice rules. 2005 , 410, 120-124		18
937	First principles calculations of thermodynamics for semiconductor alloys. 2005 , 412, 92-96		
936	Density functional study of non-polar surfaces of wurtzite CdSe. 2005 , 414, 322-325		17
935	Description of coordinatively unsaturated sites regeneration over MoS ₂ -based HDS catalysts using 35S experiments combined with computer simulations. 2005 , 289, 51-58		25
934	Density functional study of oxygen adsorption on 4- π carbon nanotubes. <i>Physical Review B</i> , 2005 , 72,	3-3	28
933	Potential super-hard phases and the stability of diamond-like boron-carbon structures. 2005 , 17, 3221-3229		56
932	Electronic properties of single-walled silicon nanotubes compared to carbon nanotubes. <i>Physical Review B</i> , 2005 , 72,	3-3	131
931	Adsorption of Ar atoms on the relaxed defect-free TiO ₂ (110) surface. <i>Physical Review B</i> , 2005 , 71,	3-3	16

930	Ab initio Ti-Zr-Ni phase diagram predicts stability of icosahedral TiZrNi quasicrystals. <i>Physical Review B</i> , 2005 , 71,	3-3	29
929	Physics of thin-film ferroelectric oxides. 2005 , 77, 1083-1130		1700
928	Application of Density Functional Theory to the Modeling of the Mixed Ionic and Electronic Conductor La ₂ NiO ₄ + δ Lattice Relaxation, Oxygen Mobility, and Energetics of Frenkel Defects. 2005 , 17, 6538-6544		67
927	Ab initio determination of electrical and thermal conductivity of liquid aluminum. <i>Physical Review B</i> , 2005 , 72,	3-3	97
926	Structure and Bonding of Li _{1.42(5)} Pd ₂ Sn _{5.58(5)} : A Lithium Intercalated Palladium Stannide. 2005 , 17, 911-915		8
925	Uniform catalytic site in Sn-beta-zeolite determined using X-ray absorption fine structure. 2005 , 127, 12924-32		119
924	Electronic structure calculations of physisorption and chemisorption on oxide glass surfaces. <i>Physical Review B</i> , 2005 , 72,	3-3	37
923	Crystal structure of Ca(AlH ₄) ₂ predicted from density-functional band-structure calculations. <i>Physical Review B</i> , 2005 , 71,	3-3	56
922	Thermodynamics of Oxides with Substitutional Disorder: A Microscopic Model and Evaluation of Important Energy Contributions. 2005 , 81, 517-525		26
921	Electronic Structure and Bonding of All Crystalline Phases in the Silica-Triple Silicon Nitride Phase Equilibrium Diagram. 2005 , 87, 1996-2013		40
920	From high resolution spectroscopy to the modeling of potential energy surfaces. 2005 , 98, 692		2
919	Band structure and the magnetic and elastic properties of SrFeO ₃ and LaFeO ₃ perovskites. 2005 , 47, 2082		62
918	Comparative analysis of the phonon modes in AgNbO ₃ and NaNbO ₃ . 2005 , 47, 2130		9
917	Optimization of the calculations of the electronic structure of carbon nanotubes. 2005 , 47, 2196		3
916	Impurities block the alpha to omega martensitic transformation in titanium. 2005 , 4, 129-33		179
915	Trans-interface diffusion-controlled coarsening. 2005 , 4, 309-16		179
914	Geometry of {001} Surfaces of Spinel (MgAl ₂ O ₄): First-Principles Simulations and Experimental Measurements. 2005 , 88, 1544-1548		30
913	Magnetoresistance and Hall effect measurements of Ni to 6GPa. 2005 , 294, 347-358		3

912	First principles calculations on Ni impurities in Cu clusters. 2005 , 294, 122-126	6
911	Magnetic and half-metallic properties of Cr-doped β -SiC. 2005 , 41, 2733-2735	12
910	Magnetic property calculations for B ₂ -Co/ _x Al/ _{1-x} structures at the interface of Co-Al multilayer. 2005 , 41, 3343-3345	1
909	Theory of tunneling magnetoresistance for epitaxial systems. 2005 , 41, 2645-2648	28
908	Accuracy and efficiency of atomic basis set methods versus plane wave calculations with ultrasoft pseudopotentials for DNA base molecules. 2005 , 26, 599-605	14
907	Testing the pairwise additive potential approximation using DFT: coadsorption of CO and N on Rh (100). 2005 , 6, 473-80	13
906	The influence of promoters and poisons on carbon monoxide adsorption on Rh(100): a DFT study. 2005 , 6, 1293-8	14
905	Phase stability and broken-symmetry transition of elemental lithium up to 140 GPa. 2005 , 6, 1703-6	38
904	Oxidation of formic acid and carbon monoxide on gold electrodes studied by surface-enhanced Raman spectroscopy and DFT. 2005 , 6, 2597-606	89
903	Density functional calculations of the reflectivity of shocked xenon with ionization based gap corrections. 2005 , 45, 300-304	33
902	SrSi ₆ N ₈ —a reduced nitridosilicate with a Si-Si bond. 2005 , 44, 567-70	35
901	Predicting new ferromagnetic nitrides from electronic structure theory: IrFe ₃ N and RhFe ₃ N. 2005 , 44, 1205-10	51
900	Prediction of novel phases of tantalum(V) nitride and tungsten(VI) nitride that can be synthesized under high pressure and high temperature. 2005 , 44, 4249-54	79
899	Catalytic hydrogenation of unsaturated aldehydes on Pt(111): understanding the selectivity from first-principles calculations. 2005 , 44, 5279-82	98
898	SrAlSiH: a polyanionic semiconductor hydride. 2005 , 44, 7269-73	44
897	SrSi ₆ N ₈ Reduced Nitridosilicate with a Si-Si Bond. 2005 , 117, 573-576	24
896	Vorhersage neuer ferromagnetischer Nitride auf der Basis von Elektronenstrukturrechnungen: IrFe ₃ N und RhFe ₃ N. 2005 , 117, 1230-1235	9
895	Synthesen bei hohem Druck und hoher Temperatur führen zu neuen Phasen von Tantal(V)-nitrid und Wolfram(VI)-nitrid. 2005 , 117, 4321-4326	6

894	Catalytic Hydrogenation of Unsaturated Aldehydes on Pt(111): Understanding the Selectivity from First-Principles Calculations. 2005 , 117, 5413-5416	14
893	SrAlSiH: A Polyanionic Semiconductor Hydride. 2005 , 117, 7435-7439	3
892	Pressure sensitivity of olivine slip systems: first-principle calculations of generalised stacking faults. 2005 , 32, 646-654	51
891	A mapping of the electron localization function for earth materials. 2005 , 32, 208-221	14
890	Electron density distribution and bond critical point properties for forsterite, Mg ₂ SiO ₄ , determined with synchrotron single crystal X-ray diffraction data. 2005 , 32, 301-313	52
889	Computer simulations in the study of gold nanowires: the effect of impurities. 2005 , 81, 1551-1558	15
888	A DFT study on the hydrated V ₂ O ₅ -TiO ₂ -anatase catalyst: stability of monomeric species. 2005 , 114, 29-37	24
887	Atomistic behaviors of Co adatom on Al (0 0 1) surface: first-principle approach. 2005 , 286, 399-404	6
886	Electronic structure and magnetism of diluted magnetic semiconductors—first principles study. 2005 , 290-291, 1408-1411	11
885	Ab initio investigation of potential indium and gallium free chalcopyrite compounds for photovoltaic application. 2005 , 66, 2019-2023	75
884	Application of computational methods to catalytic systems. 2005 , 228, 211-225	10
883	Ab initio assisted process modeling for Si-based nanoelectronic devices. 2005 , 124-125, 62-71	1
882	The relationship between adsorption and solid acidity of heteropolyacids. 2005 , 105, 134-143	27
881	Electronic structure and magnetism of chalcopyrite semiconducting CdGeP ₂ :Cr. 2005 , 359-361, 1466-1468	3
880	Structure of enantiopure and racemic alanine adlayers on Cu(1 1 0). 2005 , 574, L1-L8	96
879	Anatase and rutile surfaces with adsorbates representative of acidic and basic conditions. 2005 , 582, 173-188	101
878	Energy scaling and surface patterning of halogen-terminated Si(001) surfaces. 2005 , 591, L292-L298	7
877	Surface atomic structure and energetics of tantalum. 2005 , 598, 276-284	21

876	LEED and DFT investigation on the (2 $\bar{1}$)-S overlayer on Co(0001). 2005 , 599, 113-121	21
875	Adsorption of atomic oxygen on the Cu(100) surface. 2005 , 599, 160-172	12
874	Progress in the lithium insertion mechanism in Cu ₃ P. 2005 , 11, 36-45	18
873	Reassessment of Al-Ce and Al-Nd binary systems supported by critical experiments and first-principles energy calculations. 2005 , 36, 3269-3279	88
872	Linking first-principles energetics to CALPHAD: An application to thermodynamic modeling of the Al-Ca binary system. 2005 , 36, 5-13	37
871	Comparison of thermodynamic databases for 3xx and 6xxx aluminum alloys. 2005 , 36, 2013-2023	18
870	Diffusion of gold and native defects in mercury cadmium telluride. 2005 , 34, 868-872	5
869	Crystal quality of InN thin films grown on ZnO substrate by radio-frequency molecular beam epitaxy. 2005 , 34, 424-429	8
868	The Nature of the Catalytic Sites for H ₂ Dissociation. 2005 , 36, 55-63	9
867	Density functional theory study of alloy element interstitials in Al. 2005 , 10, 155-162	7
866	Theoretical Study of Boron Clustering in Silicon. 2005 , 4, 203-219	2
865	Electronic structure of β -Al ₂ O ₃ in the bulk and on the surface. 2005 , 48, 1127-1133	4
864	First-Principles Electronic Structure, Chemical Bonding, and High-Pressure Phase Prediction of the Oxynitrides of Vanadium, Niobium, and Tantalum. 2005 , 631, 887-893	32
863	Density functional theory calculations on microscopic aspects of oxygen diffusion in ceria-based materials. 2005 , 101, 826-839	36
862	Adsorption of 1-propanol on the Si(100) surface. 2005 , 105, 359-367	8
861	Electronic and structural properties of orthorhombic KTiOPO ₄ and related isomorphous materials. 2005 , 242, 1392-1398	9
860	Li ₂ O at high pressures: structural properties, phase-transition, and phonons. 2005 , 242, 1857-1863	39
859	Spin polarization and electronic structure of ferromagnetic Mn ₅ Ge ₃ epilayers. 2005 , 242, R67-R69	59

858	Density Functional Electronic Structure Calculations of Lithium Ion Adsorption on Defective Carbon Nanotubes. 2005 , 3, 358-361	13
857	Ab Initio Molecular Dynamics Simulations on Structural Properties of Liquid In 20 Sn 80. 2005 , 22, 1987-1990	2
856	DFT Analysis of the Indium-Antimony-Vacancy Cluster in Silicon. 2005 , 245-246, 29-38	2
855	Experimental and theoretical studies of plasma resonance and the electronic structure of binary skutterudites. 2005 , 886, 1	
854	Photoluminescence Studies on Cu and O Defects in Crystalline and Thin-film CdTe. 2005 , 865, 5241	
853	Grain boundary decohesion by impurity segregation in a nickel-sulfur system. 2005 , 307, 393-7	260
852	Electronic Structure of AgPbmSbTem+2 Compounds ¶ Implications on Thermoelectric Properties. 2005 , 886, 1	1
851	Defect Interaction Mechanisms between Antimony and Indium in Silicon. 2005 , 108-109, 425-432	
850	First-Principles Investigation of Laves Phases in Mg-Al-Ca System. 2005 , 488-489, 169-176	11
849	Oxygen Self-Diffusion Mechanisms in Silica by First-Principles. 2005 , 237-240, 115-120	
848	Theoretical Studies of Hydrogen and Water Adsorption on Actinide Oxide Surfaces. 2005 , 893, 1	2
847	A First Principles Study of Ultra-Thin (AlO)n Nanorods: Mechanical Behaviour Under Tension and Compression. 2005 , 219, 123-130	
846	Orientation and Composition Dependences of the Surface Energy and Work Function Observed by First-Principles Calculation for the Mo¶F System. 2005 , 74, 1766-1771	8
845	Ab Initio Calculation of Work Functions of ZrO/W(100) and YO/W(100) Surfaces. 2005 , 44, 7518-7520	2
844	First-Principles Calculations of Atomistic Behaviors in Ni/Al (001) and Al/Ni (001) System. 2005 , 44, 5700-5702	11
843	Atomic and electronic structure of carbon strings. 2005 , 17, 3823-36	29
842	Chirality Dependence of Mechanical Properties of Single-Walled Carbon Nanotubes under Axial Tensile Strain. 2005 , 44, L1307-L1309	28
841	Stability of the Metastable Phases in the Co¶a System Studied by ab initio and Thermodynamic Calculations Together with Ion-Beam-Mixing Experiment. 2005 , 74, 2501-2505	10

840	Layered growth modelling of epitaxial growth processes for SiC polytypes. 2005 , 17, 5355-5366		5
839	H enhancement of N vacancy migration in GaN. 2005 , 87, 201901		6
838	Doping a C60 molecule with potassium atoms: A theoretical study. 2005 , 98, 116103		
837	First-principles calculation of free Si(100) surface impurity enrichment. 2005 , 87, 232101		7
836	Molecular dissociation of group-V hydrides on Si(001). <i>Physical Review B</i> , 2005 , 72,	3-3	16
835	Coverage and strain dependent magnetization of titanium-coated carbon nanotubes. <i>Physical Review B</i> , 2005 , 71,	3-3	13
834	Jahn-Teller distortion and ferromagnetism in the dilute magnetic semiconductors GaAs:Mn and cubic GaN:Mn. <i>Physical Review B</i> , 2005 , 72,	3-3	36
833	Ab initio study of disorder broadening of core photoemission spectra in random CuPd and AgPd alloys. <i>Physical Review B</i> , 2005 , 72,	3-3	24
832	Cycloidal magnetic order in the compound IrMnSi. <i>Physical Review B</i> , 2005 , 71,	3-3	18
831	Polar phonons and intrinsic dielectric response of the ferromagnetic insulating spinel CdCr ₂ S ₄ from first principles. <i>Physical Review B</i> , 2005 , 72,	3-3	51
830	Normal mode approach for predicting the mechanical properties of solids from first principles: Application to compressibility and thermal expansion of zeolites. <i>Physical Review B</i> , 2005 , 71,	3-3	19
829	MgO addimer diffusion on MgO(100): A comparison of ab initio and empirical models. <i>Physical Review B</i> , 2005 , 72,	3-3	52
828	A first-principles study of Group IV dimer chains on Si(100). <i>Physical Review B</i> , 2005 , 72,	3-3	17
827	Binding of the N interstitial with neutral MgH in p-type GaN investigated with density functional theory. <i>Physical Review B</i> , 2005 , 72,	3-3	4
826	P-assisted growth of molecular wires on Si(001)-2 \times 1. 2005 , 86, 023108		3
825	Phase separation and charge localization in UHV-lithiated anatase TiO ₂ nanoparticles. <i>Physical Review B</i> , 2005 , 71,	3-3	14
824	Metal-semiconductor and semiconductor-semiconductor transitions in carbon nanotubes induced by intercalating alkali atoms. <i>Physical Review B</i> , 2005 , 71,	3-3	15
823	Lifting the Pt[100] surface reconstruction through oxygen adsorption: a density functional theory analysis. 2005 , 122, 184709		34

822	Real-space investigation of the metal-insulator transition of Si(557)Au. <i>Physical Review B</i> , 2005 , 72,	3-3	47
821	Electronic structure and bonding of intergranular glassy films in polycrystalline Si ₃ N ₄ : Ab initio studies and classical molecular dynamics simulations. <i>Physical Review B</i> , 2005 , 71,	3-3	35
820	Chemisorption and diffusion of hydrogen on surface and subsurface sites of flat and stepped nickel surfaces. 2005 , 122, 204707		75
819	Atomic vibrational density of states of crystalline FeSi ₂ and amorphous FeSi ₂ thin films. <i>Physical Review B</i> , 2005 , 71,	3-3	20
818	Origin of nonlocal interactions in adsorption of polar molecules on Si(001)-2 x 1. 2005 , 122, 164706		25
817	First-principles determination of exchange interactions in delafossite YCuO _{2.5} . <i>Physical Review B</i> , 2005 , 71,	3-3	22
816	Theoretical study of B diffusion with charged defects in strained Si. <i>Physical Review B</i> , 2005 , 72,	3-3	26
815	[1100][1102] twin boundaries in wurtzite ZnO and group-III-nitrides. <i>Physical Review B</i> , 2005 , 71,	3-3	24
814	Isomers of small Pbn clusters (n=2-15): Geometric and electronic structures based on ab initio molecular dynamics simulations. <i>Physical Review B</i> , 2005 , 72,	3-3	50
813	In situ revelation of a zinc-blende InN wetting layer during Stranski-Krastanov growth on GaN(0001) by molecular-beam epitaxy. <i>Physical Review B</i> , 2005 , 71,	3-3	1
812	First-principles investigations of aluminum hydrides: M ₃ AlH ₆ (M=Na,K). <i>Physical Review B</i> , 2005 , 71,	3-3	22
811	Annealing process in quenched Al-Sn alloys: A positron annihilation study. <i>Physical Review B</i> , 2005 , 71,	3-3	18
810	Spinel-type gallium oxynitrides attainable at high pressure and high temperature. <i>Physical Review B</i> , 2005 , 72,	3-3	23
809	First-order Raman spectra of AB _{1-x} B _{1+x} O ₃ double perovskites. <i>Physical Review B</i> , 2005 , 71,	3-3	80
808	Dissolution dynamics of NaCl nanocrystal in liquid water. 2005 , 72, 012602		27
807	Atom transfer and single-atom contacts. 2005 , 94, 126102		146
806	Silicon interstitials at Si/SiO ₂ interfaces: Density functional calculations. <i>Physical Review B</i> , 2005 , 72,	3-3	21
805	Observation of substitutional and interstitial phosphorus on clean Si(100)(2x1) with scanning tunneling microscopy. <i>Physical Review B</i> , 2005 , 72,	3-3	6

804	Atomic and electronic structure of the Si(001)Bb chemisorption system at 0.5 and 1.0 monolayer coverage. <i>Physical Review B</i> , 2005 , 71,	3-3	
803	Using Ar adsorption to estimate the van der Waals contribution to the wetting of Ru(0001). <i>Physical Review B</i> , 2005 , 72,	3-3	19
802	Te antisite incorporation in ZnS1xTex thin films. <i>Physical Review B</i> , 2005 , 71,	3-3	8
801	Structural, thermal, and electronic properties of Fe2VSi1-xAlx. <i>Physical Review B</i> , 2005 , 71,	3-3	22
800	Method to calculate electrical forces acting on a sphere in an electrorheological fluid. 2005 , 71, 031503		17
799	Chemically resolved scanning tunneling microscopy imaging of Al on p-type Al0.1Ga0.9As(001)-c(2x8)(2x4). 2005 , 122, 124702		1
798	Disorder and the effective MnMn exchange interaction in Ga1-xMnxAs diluted magnetic semiconductors. <i>Physical Review B</i> , 2005 , 72,	3-3	13
797	On the convergence of isolated neutral oxygen vacancy and divacancy properties in metal oxides using supercell models. 2005 , 122, 224705		23
796	Ab initio study of the effect of hydrogen and point defects on arsenic segregation at Si(100)BiO2 interfaces. 2005 , 86, 152106		9
795	Ab initio study of the adsorption of Fe atoms on a defective MgO(001) surface: Blind adsorption. <i>Physical Review B</i> , 2005 , 71,	3-3	15
794	Origin of modulated structures in YBa2Cu3O6.63: A first-principles approach. <i>Physical Review B</i> , 2005 , 71,	3-3	13
793	Construction of n-body potentials for hcp-bcc metal systems within the framework of embedded atom method. <i>Physical Review B</i> , 2005 , 71,	3-3	9
792	Surface electronic structure of Cr(001): Experiment and theory. <i>Physical Review B</i> , 2005 , 72,	3-3	28
791	Growth and structure of small gold particles on rutile TiO2(110). <i>Physical Review B</i> , 2005 , 72,	3-3	58
790	First-principles study of the effect of lattice vibrations on Cu nucleation free energy in Fe-Cu alloys. <i>Physical Review B</i> , 2005 , 72,	3-3	30
789	H placement in Cr(Mo,Fe)N supercells: The origin of the dead layers. <i>Physical Review B</i> , 2005 , 71,	3-3	9
788	Pressure induced complexity in a lithium monolayer: Ab initio calculations. <i>Physical Review B</i> , 2005 , 72,	3-3	21
787	Polarons in semiconducting polymers: Study within an extended Holstein model. <i>Physical Review B</i> , 2005 , 71,	3-3	36

786	Ab initio structural energetics of Bi_3N_4 surfaces. <i>Physical Review B</i> , 2005 , 72,	3-3	29
785	Pressure-dependent Schottky barrier at the metal-nanotube contact. 2005 , 87, 013112		12
784	Density functional calculations of Ti-enhanced NaAlH_4 . <i>Physical Review B</i> , 2005 , 71,	3-3	103
783	A density-functional study of the structural, electronic, magnetic, and vibrational properties of Ti_8C_{12} metallocarbohedrynes. 2005 , 123, 154106		19
782	Phase stability tuning in the $\text{Nb}_x\text{Zr}_{1-x}\text{N}$ thin-film system for large stacking fault density and enhanced mechanical strength. 2005 , 86, 131922		40
781	Interaction potentials from periodic density-functional theory calculations: molecular-dynamics simulations of Au clusters deposited on the TiN (001) surface. 2005 , 123, 244706		6
780	Initial stages of Ti growth on diamond (100) surfaces: from single adatom diffusion to quantum wire formation. 2005 , 94, 086101		20
779	Role of strain-dependent surface energies in Ge/Si(100) island formation. 2005 , 94, 176102		75
778	N interstitial and its interaction with substitutional Mg in p-type GaN. 2005 , 98, 033704		3
777	Effect of external electric field on the surface energetics of AgBi (111). <i>Physical Review B</i> , 2005 , 71,	3-3	15
776	Ferromagnetism of an all-carbon composite composed of a carbon nanowire inside a single-walled carbon nanotube. 2005 , 86, 163105		21
775	Ab initio theory of dynamical core-hole screening in graphite from x-ray absorption spectra. 2005 , 94, 167401		50
774	Low-temperature resistance anomaly at SrTiO_3 grain boundaries: evidence for an interface-induced phase transition. 2005 , 95, 197601		19
773	First-principles calculations of the isosteric Bain path of cobalt. <i>Physical Review B</i> , 2005 , 72,	3-3	4
772	Structure determination of indium-induced $\text{Si}(111)\sqrt{3}\times\sqrt{3}$ surface by LEED Patterson inversion. <i>Physical Review B</i> , 2005 , 72,	3-3	13
771	First-principles investigation of ferroelectricity in epitaxially strained Pb_2TiO_4 . <i>Physical Review B</i> , 2005 , 71,	3-3	20
770	Atomic and electronic structure of the (4×4) and (8×8) InBi (111) surfaces. <i>Physical Review B</i> , 2005 , 71,	3-3	24
769	Structure and dynamics of the diarsenic complex in crystalline silicon. <i>Physical Review B</i> , 2005 , 72,	3-3	8

768	Reply to Comment on Structural stability and electronic structure for Li_3AlH_6 . <i>Physical Review B</i> , 2005 , 71,	3-3	12
767	Metallic atomic wires on patterned dihydrogenated Si(001). <i>Physical Review B</i> , 2005 , 71,	3-3	7
766	First-principles study of field-emission properties of nanoscale graphite ribbon arrays. <i>Physical Review B</i> , 2005 , 72,	3-3	28
765	Top-gated field-effect transistor and rectifying diode operation of core-shell structured GaP nanowire devices. <i>Physical Review B</i> , 2005 , 71,	3-3	35
764	First-principles calculation of intrinsic defect formation volumes in silicon. <i>Physical Review B</i> , 2005 , 72,	3-3	68
763	Interaction of doping impurities with the 30° partial dislocations in SiC: An ab initio investigation. <i>Physical Review B</i> , 2005 , 72,	3-3	15
762	Magnetic doping of 4d transition-metal surfaces: A first-principles study. <i>Physical Review B</i> , 2005 , 71,	3-3	19
761	Interrupted chain-assisted Al atomic wires on Si(211): Density functional calculations. <i>Physical Review B</i> , 2005 , 72,	3-3	1
760	Electronic structure of identical metal cluster arrays on Si(111) surfaces. <i>Physical Review B</i> , 2005 , 72,	3-3	25
759	Ab initio calculation of impurity effects in copper oxide materials. <i>Physical Review B</i> , 2005 , 72,	3-3	24
758	Overcoming computational uncertainties to reveal chemical sensitivity in single molecule conduction calculations. 2005 , 122, 224502		25
757	Neutral self-defects in a silica model: A first-principles study. <i>Physical Review B</i> , 2005 , 71,	3-3	50
756	Violation of the symmetry rule for the [2+2] addition in the chemisorption of C_2H_4 on Si(100). <i>Physical Review B</i> , 2005 , 72,	3-3	32
755	Systematic pathway generation and sorting in martensitic transformations: Titanium β to α' . <i>Physical Review B</i> , 2005 , 72,	3-3	25
754	Crossover energetics for halogenated Si(100): Vacancy line defects, dimer vacancy lines, and atom vacancy lines. <i>Physical Review B</i> , 2005 , 71,	3-3	12
753	Free-energy calculations for the cubic ZrO_2 crystal as an example of a system with a soft mode. 2005 , 123, 204708		23
752	Zinc-blende half-metallic ferromagnets are rarely stabilized by coherent epitaxy. <i>Physical Review B</i> , 2005 , 71,	3-3	66
751	Density-functional studies of tungsten trioxide, tungsten bronzes, and related systems. <i>Physical Review B</i> , 2005 , 72,	3-3	85

750	Ab initio studies on the stability and electronic structure of LiCoO ₂ (003) surfaces. <i>Physical Review B</i> , 2005 , 71,	3-3	25
749	Transition from ferromagnetism to antiferromagnetism in Ga _{1-x} MnxN. 2005 , 98, 083905		16
748	Structure of GaSb digitally doped with Mn. <i>Physical Review B</i> , 2005 , 71,	3-3	7
747	Surface energy anisotropy of FePt nanoparticles. 2005 , 97, 084315		22
746	Differential tunneling spectroscopy simulations: Imaging surface states. <i>Physical Review B</i> , 2005 , 71,	3-3	32
745	Cohesive and magnetic properties of Ni, Co, and Fe on W(100), (110), and (111) surfaces: A first-principles study. <i>Physical Review B</i> , 2005 , 72,	3-3	24
744	Ab initio study of Mg(AlH ₄) ₂ . <i>Physical Review B</i> , 2005 , 72,	3-3	46
743	Rewritable Pressure-Driven n ⁺ Conduction Switching in Marcasite-Type CrSb ₂ .		0
742	Investigating the effect of pH on the growth of coprecipitated Ni _{0.8} Co _{0.1} Mn _{0.1} (OH) ₂ agglomerates as precursors of cathode materials for Li-ion batteries. 2023 ,		0
741	In situ quantitative single-molecule study of site-specific photocatalytic activity and dynamics on ultrathin g-C ₃ N ₄ nanosheets.		1
740	Tuning of Second-Harmonic Generation in Zn-Based Metal-Organic Frameworks by Controlling the Structural Interpenetrations: A First-Principles Investigation. 2023 , 127, 2058-2068		0
739	Combined ab initio and experimental screening of phase stabilities in the Ce-Fe-Ti- X system (X=3d and 4d metals). 2023 , 7,		0
738	Efficiently Light-Driven Nonoxidative Coupling of Methane on Ag/NaTaO ₃ : A Case for Molecular-Level Understanding of the Coupling Mechanism. 2023 , 13, 2094-2105		0
737	Nanoscale Iron Redistribution during Thermochemical Decomposition of CaTi _{1-x} FexO ₃ : Alters the Electrical Transport Pathway: Implications for Oxygen-Transport Membranes, Electrocatalysis, and Photocatalysis. 2023 , 6, 1620-1630		0
736	Materials synthesizability and stability prediction using a semi-supervised teacher-student dual neural network.		0
735	Revealing the electronic, optical and photocatalytic properties of PN-M ₂ CO ₂ (P = Al, Ga; M = Ti, Zr, Hf) heterostructures.		0
734	PtS ₂ /g-C ₃ N ₄ van der Waals heterostructure: A direct Z-scheme photocatalyst with high optical absorption, solar-to-hydrogen efficiency and catalytic activity. 2023 ,		0
733	Electronic transport in copper-graphene composites. 2023 , 122, 031903		0

- 732 General low-temperature growth of two-dimensional nanosheets from layered and nonlayered materials. **2023**, 14, ○
- 731 Defect and strain engineered MoS₂/graphene catalyst for an enhanced hydrogen evolution reaction. **2023**, 13, 4056-4064 ○
- 730 Raman Spectroscopy Signatures of Boron-Rich Superhard Materials from Density Functional Theory. **2023**, 127, 2104-2115 ○
- 729 Charged species redistribution at electrochemical interfaces: Model system of zirconium oxide/water interface. ○
- 728 Density functional theory study of adsorption of H₂O on $\sqrt{3}\sqrt{3}$ (110) surface. ○
- 727 Sc₂CX (X=N₂, ON, O₂) MXenes as a promising anode material: A first-principles study. **2023**, 133, 044301 ○
- 726 Vinylene carbonate reactivity at lithium metal surface: first-principles insights on the early steps of SEI formation. ○
- 725 Aluminum-doped cadmium sulfide homojunction photoelectrode with optimal film quality and water-splitting performance. ○
- 724 Automated Graph Neural Networks Accelerate the Screening of Optoelectronic Properties of Metal-Organic Frameworks. **2023**, 14, 1239-1245 ○
- 723 Chlorine Adsorption on the Ag(110) Surface: STM and DFT Study. **2023**, 127, 2266-2273 ○
- 722 Effect of vacancy defects on the electronic and mechanical properties of two-dimensional MoSi₂N₄. **2023**, 13, 5307-5316 ○
- 721 From High-Entropy Alloys to High-Entropy Ceramics: The Radiation-Resistant Highly Concentrated Refractory Carbide (CrNbTaTiW)_{1-x}C. ○
- 720 Learning local equivariant representations for large-scale atomistic dynamics. **2023**, 14, 1 ○
- 719 The Stability of a Mixed-Phase Barium Cerium Iron Oxide under Reducing Conditions in the Presence of Hydrogen. **2023**, 28, 1429 ○
- 718 Siloxane Molecules: Nonlinear Elastic Behavior and Fracture Characteristics. ○
- 717 Spin-crossover in [Fe(Quinazoline)₂][Fe(CN)₅NO]. Evidence of its framework flexibility. **2023**, 549, 121402 ○
- 716 Sign change of anomalous Hall effect and anomalous Nernst effect in the Weyl semimetal CeAlSi. **2023**, 107, ○
- 715 Noble-metal single atom with non-metal co-doped graphene: First-principles investigation of structures, electronic and magnetic properties. **2023**, 568, 170418 ○

- 714 Interplay of magnetic and electric coupling across the spin density wave to conical magnetic ordering in a BaHoFeO₄ spin-cluster chain compound. **2023**, 942, 169017 ○
- 713 Band gap tailoring in a low toxicity and low-cost solar cell absorber Cu₃SbS₄ through Na alloying: a first-principles study. **2023**, 127132 ○
- 712 LAVA 1.0: A general-purpose python toolkit for calculation of material properties with LAMMPS and VASP. **2023**, 286, 108667 ○
- 711 Reaching the initial coulombic efficiency and structural stability limit of P2/O3 biphasic layered cathode for sodium-ion batteries. **2023**, 638, 758-767 ○
- 710 SrCuP and SrCuSb Zintl phases as potential thermoelectric materials. **2023**, 942, 169123 ○
- 709 Study of Workload Interference with Intelligent Routing on Dragonfly. **2022**, ○
- 708 2.5 Million-Atom Ab Initio Electronic-Structure Simulation of Complex Metallic Heterostructures with DGDF. **2022**, ○
- 707 Ag-doped Pd nano-dendritic for promoting the electrocatalytic oxidation of ethylene to ethylene glycol. **2023**, 7, 1437-1445 ○
- 706 SENSITIVE ELEMENTS OF TEMPERATURE CONVERTERS BASED ON HfNi_{1-x}Cu_xSn THERMOMETRICAL MATERIAL. **2023**, 84, 11-17 ○
- 705 First principles calculation of the ZnV₂O₆(001) surface terminations: the thermodynamics stability and electronic structure study. ○
- 704 Oxygen migration performance of LaFeO₃ perovskite-type oxygen carriers with Sr doping. **2023**, 25, 9216-9224 ○
- 703 First-principles study on electronic states of In₂Se₃/Au heterostructure controlled by strain engineering. **2023**, 13, 11385-11392 ○
- 702 The PdBi₂ monolayer for efficient electrocatalytic NO reduction to NH₃: a computational study. ○
- 701 Enabling triferroics coupling in breathing kagome lattice Nb₃X₈ (X = Cl, Br, I) monolayers. ○
- 700 Electron-phonon coupling, bipolar effect, and thermoelectric performance of the CuSbS₂ monolayer. ○
- 699 Ni-Intercalation-Induced Topological Nodal Line States and Superconductivity in NiTe. **2023**, 127, 4303-4309 ○
- 698 Quantum Oscillation and Electronic Structure of Sn₄As₃ and Sn₄P₃. **2023**, 127, 4319-4325 ○
- 697 Corrosiveness of Li₂TiO₃ ceramic tritium breeder to structural RAFM steel: Effects on microstructure and thermal conductivity. **2023**, ○

- 696 Inter-quintuple layer coupling and topological phase transitions in the chalcogenide topological insulators. **2023**, 5, 015001 ○
- 695 Advanced Design of Metal Nanoclusters and Single Atoms Embedded in C 1 N 1 -Derived Carbon Materials for ORR, HER, and OER. 2300405 1
- 694 Customized reaction route for ruthenium oxide towards stabilized water oxidation in high-performance PEM electrolyzers. **2023**, 14, ○
- 693 Nonharmonic contributions to the high-temperature phonon thermodynamics of Cr. **2023**, 107, ○
- 692 Temperature-Dependent Anharmonic Phonons in Quantum Paraelectric KTaO₃ by First Principles and Machine-Learned Force Fields. **2023**, 6, ○
- 691 High photostrictive efficiency of Mg₃V₂O₈ ceramics under visible light illumination. **2023**, 106, 3584-3593 ○
- 690 Impedance modeling for excluding contact resistance from cross-plane electronic conductivity measurement of anisotropic two-dimensional Ti₃C₂T_x MXenes. **2023**, 133, 065304 ○
- 689 Structure and Optical Properties of Polymeric Carbon Nitrides from Atomistic Simulations. **2023**, 35, 1547-1559 ○
- 688 Defect-Engineering of 2D Dichalcogenide VSe₂ to Enhance Ammonia Sensing: Acumens from DFT Calculations. **2023**, 13, 257 ○
- 687 Catalytic performance of binary transition metal sulfide FeCoS₂/rGO for lithium-sulfur batteries. **2023**, 27, 1045-1053 ○
- 686 Graphynes and Graphdiynes for Energy Storage and Catalytic Utilization: Theoretical Insights into Recent Advances. ○
- 685 Modeling car-following behavior in heterogeneous traffic mixing human-driven, automated and connected vehicles: considering multitype vehicle interactions. ○
- 684 On the limitations of thermal atomic layer deposition of InN using ammonia. **2023**, 41, 020401 ○
- 683 Computational Design of a Two-Dimensional Copper Carbide Monolayer as a Highly Efficient Catalyst for Carbon Monoxide Electroreduction to Ethanol. **2023**, 15, 13033-13041 ○
- 682 Simulation studies of secondary electron yield with electron transport from Cu (110) surfaces containing C₂, N₂, CO₂, or NO₂ adsorbates. 10, ○
- 681 First-principles theory of the pressure-induced invar effect in FeNi alloys. **2023**, 107, ○
- 680 First-Principles Investigation on Phase Stability, Mechanical Properties, Bonding Characteristic and Slip Properties of Ti-Co Binary Intermetallic Compounds. **2023**, 13, 628 ○
- 679 Incorporation and migration of xenon in uranium-plutonium mixed nitride; A density functional theory study. **2023**, 577, 154330 ○

- 678 Metal-Support Interactions in Heterogeneous Catalysis: DFT Calculations on the Interaction of Copper Nanoparticles with Magnesium Oxide. **2023**, 8, 10591-10599 ○
- 677 Type-II van der Waals heterostructures of GeC, ZnO and Al₂SO monolayers for promising optoelectronic and photocatalytic applications. **2023**, ○
- 676 Modeling laser interactions with aluminum and tantalum targets using a hybrid atomistic-continuum model. **2023**, 133, 105901 ○
- 675 Mechanistic Insight into Solution-Based Atomic Layer Deposition of CuSCN Provided by In Situ and Ex Situ Methods. ○
- 674 Optical Properties and Metal-Dependent Charge Transfer in Iodido Pentelates. ○
- 673 Cu dopant triggered Fe-N-C catalysts toward high efficiency electroreduction of CO₂ to CO. **2023**, 70, 102420 ○
- 672 Methane pyrolysis and carbon formation mechanisms in molten manganese chloride mixtures. **2023**, 336, 120810 ○
- 671 Strain engineering of type-II C₂N/WS₂ van der Waals heterojunction for highly enhanced photocatalytic hydrogen evolution. **2023**, ○
- 670 Phase engineering of layered anode materials during ion-intercalation in Van der Waal heterostructures. **2023**, 13, ○
- 669 Interfacial electronic states and self-formed asymmetric Schottky contacts in polar α -In₂Se₃/Au contacts. ○
- 668 Assessing Factors that Determine Adatom Migration and Clustering on a Thin Film Oxide; Pt₁ and Rh₁ on the α -Cu_xO/Cu(111) Surface. **2023**, 157145 ○
- 667 Moisture-Tailored 2D Dion-Jacobson Perovskites for Reconfigurable Optoelectronics. ○
- 666 Efficient atomistic simulations of radiation damage in W and W/Mo using machine-learning potentials. **2023**, 577, 154325 ○
- 665 Monovacancy-hydrogen interaction in pure aluminum: Experimental and ab-initio theoretical positron annihilation study. **2023**, 248, 118770 ○
- 664 cmtj: Simulation package for analysis of multilayer spintronic devices. **2023**, 9, ○
- 663 Interfacial Chemistry in the Electrocatalytic Hydrogenation of CO₂ over C-Supported Cu-Based Systems. 5876-5895 ○
- 662 Spin and current transport in the robust half-metallic magnet δ -CoFeGe. ○
- 661 Gate switchable spin-orbit splitting in a MoTe₂/WTe₂ heterostructure from first-principles calculations. **2023**, 107, ○

- 660 Characterization of Planar Defect in Layered Perovskite Photocatalyst Y₂Ti₂O₅S₂ by Electron Microscopy and First-Principles Calculations. ○
- 659 High-precision measurements and first-principles explanation of the temperature-dependent C13 and N14. **2023**, 107, ○
- 658 Enhancing the accuracy of density functional tight binding models through CHIMES many-body interaction potentials. **2023**, 158, 144112 ○
- 657 Stable Two Dimensional Na Decorated BeN₄: A Potential Candidate for Hydrogen Storage. ○
- 656 Deforming lanthanum trihydride for superionic conduction. **2023**, 616, 73-76 ○
- 655 Interface alloying design to improve the stability and cohesion of W/HfC interface by first-principles study. **2023**, 577, 154320 ○
- 654 Atomic structure and bonding in fluorinated graphite intercalated with a strong fluoroxidant. **2023**, 135, 109851 ○
- 653 Gas sensing potential of monolayer MoB: A first principles study. **2023**, 210, 111883 ○
- 652 Competing spin fluctuations in Sr₂RuO₄ and their tuning through epitaxial strain. **2023**, 107, ○
- 651 Stability and Thermoelectric Properties of FeZrTe Alloy. ○
- 650 Unconstrained Machine Learning Screening for New Li-Ion Cathode Materials Enhanced by Class Balancing. ○
- 649 Thermal atomic layer etching of cobalt using plasma chlorination and chelation with hexafluoroacetylacetone. **2023**, 619, 156751 ○
- 648 Single-atom Pt supported on non-metal doped WS₂ for photocatalytic CO₂ reduction: a first-principles study. **2023**, 157252 ○
- 647 The effect of alkyl chain length on imidazole chloroaluminate ionic liquid/Pt(1 1 1) interface and aluminum deposition: A DFT-D3 study. **2023**, 568, 111842 ○
- 646 Influence of molybdenum doping on the structural, electrical, and optical properties of germanium telluride thin films. **2023**, 24, 2538-2549 ○
- 645 Promising high temperature thermoelectric performance of layered oxypnictide YZnAsO. **2023**, 657, 414811 ○
- 644 Magnetic and transport properties of two-dimensional ferromagnet VSe₂ with Se vacancies. **2023**, 574, 170683 ○
- 643 Experimental and theoretical revelation of a unique band topology in Sb₂Te₃ topological insulator by substitution of Cu high pressure stud. **2023**, 290, 116347 ○

- 642 Magnetic, optoelectronic, and rietveld refined structural properties of Al³⁺ substituted nanocrystalline Ni-Cu spinel ferrites: An experimental and DFT based study. **2023**, 573, 170675 ○
- 641 Electronic and optical properties of transition-metal (TM=Sc, Ni, Cu, Zn) adsorbed monolayer SnSe₂. **2023**, 177, 207548 ○
- 640 Prediction of superior thermoelectric performance in unexplored doped-BiCuSeO via machine learning. **2023**, 229, 111868 ○
- 639 Size-Selected Cu₄ cluster anchored on C₂N monolayer for efficient nitrite electroreduction to ammonia: a computational study. **2023**, 620, 156825 ○
- 638 Built-in electric field-assisted W-C₃/X-C₃ van der Waals heterogeneous single-atom catalysts for enhanced electrocatalytic nitrogen reduction. **2023**, 619, 156790 ○
- 637 Al₂O₃/ZnO composite-based sensors for battery safety applications: An experimental and theoretical investigation. **2023**, 109, 108301 ○
- 636 Diffusion-assisted displacive transformation in Yttrium-doped Sb₂Te₃ phase change materials. **2023**, 249, 118809 ○
- 635 States of Pt/CeO₂ catalysts for CO oxidation below room temperature. **2023**, 421, 285-299 1
- 634 In-plane adjustment of atomic positions and layer-dependent friction in 2D materials. **2023**, 620, 156810 ○
- 633 The ill-defined (AlFeMgSi) phase intermetallics formed in an automotive Al-Si-Mg alloy. **2023**, 199, 112839 ○
- 632 Design of enhanced porous organic cage solubility in Type 2 porous liquids. **2023**, 377, 121536 ○
- 631 Prediction of new stable crystal structures for ternary ErAgTe₂ and YAgTe₂ semiconductors: Ab initio study. **2023**, 139, 107160 ○
- 630 Thermal resistance from non-equilibrium phonons at SiTe interface. **2023**, 34, 101063 ○
- 629 Controlling of Localization by Elemental-substitution Effect in Layered BiCh₂-based Compounds LaO_{1-x}F_xBiS_{2-y}Se_y. **2023**, 92, ○
- 628 First principles study of oxygen diffusion in plutonium dioxide, sesquioxide, and their interface under activated conditions. **2023**, 578, 154348 ○
- 627 An exceptionally strong, ductile and impurity-tolerant austenitic stainless steel prepared by laser additive manufacturing. **2023**, 250, 118868 ○
- 626 Boron nitride as an all-in-one gelator to immobilize concentrated sulfone electrolyte towards high performance lithium metal batteries. **2023**, 59, 102753 ○
- 625 Intriguing optical and photocatalytic properties of pentagonal penta-PtPS, -PtPSe and -PtPTE monolayers: A first-principle study. **2023**, 177, 111280 ○

- 624 Unraveling the ferroelectric switching mechanisms in ferroelectric pure and La doped HfO₂ epitaxial thin films. **2023**, 34, 101064 ○
- 623 Automated calculations of exchange magnetostriction. **2023**, 224, 112158 ○
- 622 Van der Waals stacking-induced efficient Ohmic contacts and the weak Fermi level pinning effect in MoSi₂N₄ and WSi₂N₄ contact with two-dimensional metals. **2023**, 149, 115686 1
- 621 Dual MOF-derived Fe/N/P-tridoped carbon nanotube as high-performance oxygen reduction catalysts for zinc-air batteries. **2023**, 327, 122469 ○
- 620 On the enhanced performance of Pt-based high-entropy alloys catalyst during water-gas shift reaction: A density functional theory study. **2023**, 623, 157023 ○
- 619 High temperature elastic properties of sub-stoichiometric yttrium dihydrides. **2023**, 35, 105879 ○
- 618 High throughput screening of single atomic catalysts with optimized local structures for the electrochemical oxygen reduction by machine learning. **2023**, 81, 349-357 ○
- 617 Machine learning insight into h-BN growth on Pt(111) from atomic states. **2023**, 621, 156893 ○
- 616 2D Mg₂M₂X₅ (M = B, Al, Ga, In, Tl; X = S, Se, Te) monolayers: Novel stable semiconductors for water splitting photocatalysts. **2023**, 621, 156892 ○
- 615 Unraveling the role of defect types in Fe₃O₄ for efficient NIR-driven photocatalytic inactivation. **2023**, 622, 156860 ○
- 614 ZIF-67 derived Mo-CoS₂ nanoparticles embedded in hierarchically porous carbon hollow sphere for efficient overall water splitting. **2023**, 623, 157030 ○
- 613 Through the Self-Optimization process to achieve high OER activity of SAC catalysts within the framework of TMO₃@G and TMO₄@G: A High-Throughput theoretical study. **2023**, 640, 405-414 ○
- 612 First principles investigation on electronic structure, elasticity, thermodynamic properties of H-Cu₂As₂O₇. **2023**, 292, 116371 ○
- 611 Towards the understanding of (dis)charging mechanism of VS₄ cathode for magnesium batteries. **2023**, 62, 106895 ○
- 610 VTAnDeM: A python toolkit for simultaneously visualizing phase stability, defect energetics, and carrier concentrations of materials. **2023**, 287, 108691 ○
- 609 First-principles calculations integrated with experimental optical and electronic properties for MoS₂-graphene heterostructures and MoS₂-graphene-Au heterointerfaces. **2023**, 623, 156948 ○
- 608 Electrocatalytic reduction of carbon dioxide in confined microspace utilizing single nickel atom decorated nitrogen-doped carbon nanospheres. **2023**, 111, 108384 ○
- 607 The effects of mixing non-metal atoms in the B1 structured transition metal carbo-nitrides on their structure and mechanical properties: HfC₁-N. **2023**, 14, 100356 ○

- 606 Machine Learning for the edge energies of high symmetry Au nanoparticles. **2023**, 732, 122265 ○
- 605 The adjustable electronic and photoelectric properties of the WS₂/WSe₂ and WSe₂/WTe₂ van der Waals heterostructures. **2023**, 212, 112020 ○
- 604 First-principles studies the optical properties of defective-GQDs and -fullerene. **2023**, 35, e00793 ○
- 603 Computational screening of B borophene based single-atom catalysts for N₂ reduction. **2023**, 418, 114079 ○
- 602 The optical properties of In₂S₃ films in the far-infrared spectral range. **2023**, 131, 104662 ○
- 601 Effects of uniaxial strain on elastic and electronic properties of hydrogenated XC (X=Si, Ge, and Sn) monolayers by first-principles calculations. **2023**, 472, 128808 ○
- 600 First-principles study on electronic structure and thermodynamic stability of two-dimensional pentagonal MX₂ (M = Pd, Pt; X = S, Se, Te). **2023**, 212, 111982 ○
- 599 Evaluation of battery positive-electrode performance with simultaneous ab-initio calculations of both electronic and ionic conductivities. **2023**, 569, 232969 ○
- 598 Epitaxially strained ultrathin LaNiO₃/LaAlO₃ and LaNiO₃/SrTiO₃ superlattices: A density functional theory + U study. **2023**, 50, 53-60 ○
- 597 Heterogeneous nucleation of carbides attached to Y₂O₃ in Y-modified H13 steel. **2023**, 200, 112891 ○
- 596 First-principles investigations of the crystal and electronic structures, dynamical and mechanical stabilities, Born effective charges and dielectric permittivities of a novel tetragonal zirconia. **2023**, 659, 414862 ○
- 595 Crucial role of alkali metal ions and Si/Al ratio in selective adsorption of 1-octene using faujasite zeolites. **2023**, 314, 123531 ○
- 594 Insights into the enhanced performance of NiCo-LDH modified Pd/NF cathode for electrocatalytic hydrodechlorination. **2023**, 341, 127689 ○
- 593 Short bandgap of porphyrin molecules (Py) filled in a semiconducting single-walled carbon nanotube (Py@NT17) for highly efficient organic photovoltaic cells. **2023**, 293, 116456 ○
- 592 Theoretical approach to the one-step versus two-step spin transitions in Hofmann-like Fell SCO metal-organic frameworks. **2023**, 30, 101489 ○
- 591 Ti-decorated nitrogen-rich BeN₄ monolayer for reversible hydrogen storage: DFT investigations. **2023**, 622, 156806 ○
- 590 Ir-trimer anchored on the Co-supported Pd nanocrystals Opens the Ultra-efficient Channel on oxygen reduction reaction. **2023**, 622, 156857 ○
- 589 The hinge morphology of SnO₂ as multifunctional semiconductor: What we can learn from simulations, theory, and experiments. **2023**, 622, 156904 ○

- 588 Prediction of novel final phases in aged uranium-niobium alloys. **2023**, 579, 154394 ○
- 587 Two-dimensional van der Waals layered VSi₂N₄ as anode materials for alkali metal (Li, Na and K) ion batteries. **2023**, 178, 111339 ○
- 586 Defect engineered Janus MoSiGeN₄ as highly efficient electrocatalyst for hydrogen evolution reaction. **2023**, 622, 156894 ○
- 585 Ion diffusion, and hysteresis of magnesium hydride conversion electrode materials. **2023**, 155, 47-53 1
- 584 Free-templated synthesis of N-doped PtCu porous hollow nanospheres for efficient ethanol oxidation and oxygen reduction reactions. **2023**, 330, 122602 ○
- 583 Atomic-scale engineering of cation vacancies in two-dimensional unilamellar metal oxide nanosheets for electricity generation from water evaporation. **2023**, 110, 108348 ○
- 582 Electronic modulation with Pt-incorporated NiFe layered double hydroxide for ultrastable overall water splitting at 1000 mA cm⁻². **2023**, 331, 122683 ○
- 581 Structural and photoluminescence properties of Co-Sputtered p-type Zn-doped Ga₂O₃ thin films on sapphire substrates. **2023**, 260, 119836 ○
- 580 Noble metal single-atoms for lithium-ion batteries: A booster for ultrafast charging/discharging in carbon electrodes. **2023**, 624, 157161 ○
- 579 Influence of solution-hardening on the mechanical properties and wear resistance of copper alloys. **2023**, 523, 204869 ○
- 578 Experimental and computational study on the C15 phase structure stability of Y Ni₂-Mn system. **2023**, 952, 169632 ○
- 577 Design, synthesis and investigating the interaction of novel s-triazine collector with pyrite surface: A DFT-D3+U and experimental studies. **2023**, 38, 102820 ○
- 576 Concentration effects on the microstructures and electronic features of Nd_xY_{1-x}AlO₃ crystals: A first-prin. **2023**, 225, 112178 ○
- 575 Electronic excitation induced non-thermal phase transition of tungsten. **2023**, 952, 170087 ○
- 574 Efficacy of pyrostitpnite (Ag₃SbS₃) mineral as thermoelectric material: A first principles study. **2023**, 162, 107513 ○
- 573 Reaction-driven evolutions of Pt states over Pt-CeO₂ catalysts during CO oxidation. **2023**, 330, 122662 ○
- 572 Dual-atom Co-Fe catalysts for oxygen reduction reaction. **2023**, 46, 48-55 ○
- 571 Nanoscale Periodic Trapping Sites for Interlayer Excitons Built by Deformable Molecular Crystal on 2D Crystal. ○

- 570 Rational design of heterogenized molecular phthalocyanine hybrid single-atom electrocatalyst towards two-electron oxygen reduction. **2023**, 14, ○
- 569 Non-precious metal single-atom loading and further strain engineering on SrTiO₃ (100) surface for optimizing hydrogen evolution reaction. **2023**, 656, 119131 ○
- 568 Highly Enhanced Chloride Adsorption Mediates Efficient Neutral CO₂ Electroreduction over a Dual-Phase Copper Catalyst. ○
- 567 3D microstructure evolution in Na_xFePO₄ storage particles for sodium-ion batteries. **2023**, 565, 232902 ○
- 566 Theoretical insights into nonmetal-doped graphyne-supported noble metal electrocatalysts for NH₃ synthesis via nitrogen reduction. **2023**, 617, 156550 ○
- 565 High-throughput screening of H₂ production catalysts from doped In₂SSe monolayer: Valence electrons-based descriptor. **2023**, 224, 112179 ○
- 564 Structural incorporation of iron influences biomethylation potential of mercury sulfide. **2023**, 349, 115-125 ○
- 563 Tunable valley characteristics of WSe₂ and WSe₂/VSe₂ heterostructure. **2023**, 624, 157111 ○
- 562 CeO₂ promotes electrocatalytic formic acid oxidation of Pd-based alloys. **2023**, 948, 169665 ○
- 561 Heterojunction material BiYO₃/g-C₃N₄ modified with cellulose nanofibers for photocatalytic degradation of tetracycline. **2023**, 312, 120829 ○
- 560 Syngas-to-Hydrocarbons on the transition metal catalysts: Revealing the function of surface hydroxyl intermediate served as co-adsorbed promoter or hydrogenating species. **2023**, 343, 127967 ○
- 559 Coordination-number-determined activity of copper catalyst in water-gas shift reaction. **2023**, 343, 127850 1
- 558 Sub-micron-sized hafnium (Hf) cathode with excellent thermal emission performance and superior hardness synthesized by powder metallurgy route. **2023**, 231, 115436 ○
- 557 Single domain Co₂FeGa nanoparticles with high crystalline order synthesized by template-less chemical method. **2023**, 949, 169848 ○
- 556 Toughness enhancement mechanism of Ni-doped Cr₂N. **2023**, 949, 169854 ○
- 555 Development of metal-organic framework-derived NiMo-MoO₃ porous nanorod for efficient electrocatalytic hydrogen evolution reactions. **2023**, 328, 122421 1
- 554 Hydrogen diffusion on the tin-covered tungsten surface: A first-principles study. **2023**, 577, 154282 1
- 553 Revealing the bifunction mechanism of LaCoO₃ as electrocatalyst: Oxygen vacancies effect and synergistic reaction process. **2023**, 941, 168918 ○

- 552 C60 surface-supported TM@Si16 (TM = Ti, Zr, Hf) superatoms as self-assembled photocatalysts. **2023**, 616, 156465 ○
- 551 Growth morphology and magnetic properties of Gd adatoms on h-BN template: From single atom to small cluster and monolayer. **2023**, 616, 156476 ○
- 550 First-principles assessment of chemical lithiation of sulfide solid electrolytes and its impact on their transport, electronic and mechanical properties. **2023**, 560, 232689 ○
- 549 Mechanistic understanding of N₂ activation: a comparison of unsupported and supported Ru catalysts. ○
- 548 First-principles study of noble metal atom doped Fe(100) as electrocatalysts for nitrogen reduction reaction. **2023**, 297, 127396 ○
- 547 Interplay of dopant and polarons in trifunctional semimagnetic semiconductor for supercapacitor applications: Local structure and electronic structure investigations. **2023**, 60, 106655 ○
- 546 First-principal investigations of the electronic, magnetic, and thermoelectric properties of CrTiRhAl quaternary Heusler alloy. **2023**, 568, 170421 ○
- 545 Structural features, thermal stability and catalytic implication of FeNi nanoparticles. **2023**, 320, 123863 ○
- 544 Theoretical and Empirical Insight into Dopant, Mobility and Defect States in W Doped Amorphous In₂O₃ for High-Performance Enhancement Mode BEOL Transistors. **2022**, ○
- 543 The combined effects of Mg²⁺ and Sr²⁺ incorporation during CaCO₃ precipitation and crystal growth. **2023**, 345, 16-33 ○
- 542 Emergence of metallic surface states and negative differential conductance in thin FeSi₂ films on Si(001). **2023**, 35, 135001 ○
- 541 CO₂ dissociation and hydrogenation on pure and Ni-doped Fe(1 1 1). A DFT theoretical approach. **2023**, 617, 156569 ○
- 540 Insights into the synergy of platinum and nickel carbonate hydroxide for efficient methanol electro-oxidation. **2023**, 616, 156587 ○
- 539 First principle study on high-entropy perovskites Ca(Ti_{0.25}Zr_{0.25}Hf_{0.25}Sn_{0.25})O₃ and Ca(Ti_{0.25}Zr_{0.25}Hf_{0.25}Ce_{0.25})O₃ as thermal barrier coatings. **2023**, 297, 127460 ○
- 538 Electrocatalytic nitrogen fixation performance of two-dimensional Metal-Organic Frameworks Cu₃(C₆O₆) and TM/Cu₃(C₆O₆) from first-principle study. **2023**, 568, 111837 ○
- 537 First-principles prediction of two-dimensional MnOX (X = Cl, Br) monolayers: the half-metallic multiferroics with magnetoelastic coupling. **2023**, 15, 4546-4552 ○
- 536 The local structure and electronic properties of Ho³⁺-doped BaY₂F₈: A first-principles method. **2023**, 298, 127459 ○
- 535 Recent advances in the ab initio theory of solid-state defect qubits. **2023**, 12, 359-397 1

- 534 First-principles calculations to investigate electronic band structure, optical and mechanical properties of new CaFCl monolayer. **2023**, 45, 106251 ○
- 533 Direct seawater electrolysis by adjusting the local reaction environment of a catalyst. **2023**, 8, 264-272 1
- 532 Two-dimensional conjugated metal-organic frameworks TM₃(HAT)₂: a new family of promising single-atom electrocatalysts for efficient nitrogen fixation. **2023**, 10, 024002 ○
- 531 Superconducting state of the van der Waals layered PdH₂ structure at high pressure. **2023**, ○
- 530 Pure Blue Perovskites Nanocrystals in Glass: Ultrafast Laser Direct Writing and Bandgap Tuning. 2200902 ○
- 529 Enhancing dehydrogenation performance of MgH₂/graphene heterojunctions via noble metal intercalation. **2023**, ○
- 528 Grain refinement in titanium prevents low temperature oxygen embrittlement. **2023**, 14, ○
- 527 Theoretical Calculations on Metal Catalysts Toward Water-Gas Shift Reaction: a Review. ○
- 526 Fast ion-conductive electrolyte based on a doped LaAlO₃ with an amorphous surface layer for low-temperature solid oxide fuel cells. **2023**, 561, 232723 ○
- 525 Unlocking AlN Piezoelectric Performance with Earth-Abundant Dopants. **2023**, 9, ○
- 524 Surface-Enhanced Raman Spectroscopy (SERS) Chemical Enhancement in the Vibronically Coupled Langmuir Layer of Mixed Dichalcogenide 1T-MoSSe with Adsorbed R6G. **2023**, 127, 3131-3141 ○
- 523 Negative piezoelectricity and enhanced electrical conductivity at the interfaces of two-dimensional dialkali oxide and chalcogenide monolayers. **2023**, 107, ○
- 522 Voltage-Controlled Dzyaloshinskii-Moriya Interaction Torque Switching of Perpendicular Magnetization. **2023**, 130, 1
- 521 DFT+U study of electronic and optical properties of Cu₃TMTe₄: TM = V, Nb, Ta with incorporation of SOC. **2023**, ○
- 520 Highly Stable Electrochemical Supercapacitor Performance of Self-Assembled Ferromagnetic Q-Carbon. **2023**, 15, 8305-8318 1
- 519 High-Temperature Thermoelectricity in Narrow-Gap Semiconductor SmS with Strong Electron-Hole Asymmetry. **2023**, 13, 2203519 ○
- 518 Band gap engineering of anatase TiO₂ by ambipolar doping: A first principles study. **2023**, 299, 127467 ○
- 517 Accurate description of hydrogen diffusivity in bcc metals using machine-learning moment tensor potentials and path-integral methods. **2023**, 247, 118739 ○

- 516 Probing the Mysterious Behavior of Tungsten as a Dopant Inside Pristine Cobalt-Free Nickel-Rich Cathode Materials. **2023**, 33, ○
- 515 Pressure tuning of structure, magnetic frustration, and carrier conduction in the Kitaev spin liquid candidate Cu_2IrO_3 . **2023**, 107, ○
- 514 Giant Rashba effect and nonlinear anomalous Hall conductivity in a two-dimensional molybdenum-based Janus structure. **2023**, 107, ○
- 513 Million-scale data integrated deep neural network for phonon properties of heuslers spanning the periodic table. **2023**, 9, ○
- 512 How Adsorption Affects the Energy Release in an Azothiophene-Based Molecular Solar-Thermal System. **2023**, 14, 1470-1477 ○
- 511 Phonon transport in Cu_2GeSe_3 : Effects of spin-orbit coupling and higher-order phonon-phonon scattering. **2023**, 107, ○
- 510 Electronic structure analysis of light-element-doped anatase TiO_2 using all-electron GW approach. **2023**, 220, 112059 ○
- 509 Fischer Esterification of Benzoic Acid and Polyhydric Alcohols Catalyzed by Basic Ionic Liquids of Bisimidazolium Tungstates. **2023**, 8, ○
- 508 Synthesis of technetium hydride $\text{TcH}_{1.3}$ at 27 GPa. **2023**, 107, ○
- 507 Role of electronic correlations in the kagome-lattice superconductor LaRh_3B_2 . **2023**, 107, ○
- 506 Role of solvation model on the stability of oxygenates on Pt(111): A comparison between microsolvation, extended bilayer, and extended metal/water interface. ○
- 505 Interplay between H-bonding proton dynamics and Fe valence fluctuations in $\text{Fe}_3(\text{PO}_4)_2(\text{OH})$. **2023**, 107, ○
- 504 Vibrational, thermodynamic and acoustic properties of AgAlS_2 crystal. **2023**, 654, 414731 ○
- 503 Hidden Zeeman-type spin polarization in bulk crystals. **2023**, 107, ○
- 502 Strain enhanced magnetism of V-implanted CrI_3 monolayer. **2023**, 122, 063101 ○
- 501 Supercapacitor Performance of Magnetite Nanoparticles Enhanced by a Catecholate Dispersant: Experiment and Theory. **2023**, 28, 1562 ○
- 500 In Silico High-Throughput Design and Prediction of Structural and Electronic Properties of Low-Dimensional Metal-Organic Frameworks. ○
- 499 Comparative study of first-principles approaches for effective Coulomb interaction strength U_{eff} between localized f-electrons: Lanthanide metals as an example. **2023**, 158, 084108 ○

- 498 Dispersed surface Ru ensembles on MgO(111) for catalytic ammonia decomposition. **2023**, 14, ○
- 497 Finding stable multi-component materials by combining cluster expansion and crystal structure predictions. **2023**, 9, ○
- 496 Atomic Scaled Depth Correlation to the Oxygen Reduction Reaction Performance of Single Atom Ni Alloy to the NiO₂ Supported Pd Nanocrystal. **2023**, 10, ○
- 495 Achieving Record-High Photoelectrochemical Photoresponse Characteristics by Employing Co₃O₄ Nanoclusters as Hole Charging Layer for Underwater Optical Communication. **2023**, 17, 3901-3912 ○
- 494 Pressure-tuning domain-wall chirality in noncentrosymmetric magnetic Weyl semimetal CeAlGe. **2023**, 66, ○
- 493 Scalable manufacturing of quantum light emitters in silicon under rapid thermal annealing. **2023**, 31, 8352 ○
- 492 Magnetic-field switching of second-harmonic generation in noncentrosymmetric magnet Eu₂MnSi₂O₇. **2023**, 7, ○
- 491 Increased localization of Majorana modes in antiferromagnetic chains on superconductors. **2023**, 107, ○
- 490 Structure-activity relationship of Cu-based catalysts for the highly efficient CO₂ electrochemical reduction reaction. 11, ○
- 489 A comparative ab initio study of acetylene activation over Au₉ cluster and Au₉ supported over ZnO monolayer. **2023**, 1222, 114072 ○
- 488 Topological spin textures in 1T -phase Janus magnets: Interplay between Dzyaloshinskii-Moriya interaction, magnetic frustration, and isotropic higher-order interactions. **2023**, 107, 1
- 487 X-ray Absorption Spectroscopy Studies of a Molecular CO₂-Reduction Catalyst Deposited on Graphitic Carbon Nitride. **2023**, 127, 3626-3633 ○
- 486 Structural Significance of Hydrophobic and Hydrogen Bonding Interaction for Nanoscale Hybridization of Antiseptic Miramistin Molecules with Molybdenum Disulfide Monolayers. **2023**, 28, 1702 ○
- 485 Origins of Electrical Compensation in Si-Doped HVPE GaN. 2200568 ○
- 484 A Two-in-one host for High-loading cathode and Dendrite-free anode realized by activating metallic nitrides heterostructures toward Li-S full batteries. **2023**, 460, 141862 ○
- 483 Pyridinic-nitrogen on ordered mesoporous carbon: A versatile NAD(P)H mimic for borrowing-hydrogen reactions. **2023**, 419, 80-98 ○
- 482 Two-Dimensional Ferroelectricity in a Single-Atom Adsorbed BiI₃ Monolayer. **2023**, 127, 3898-3903 ○
- 481 Anisotropic topological surface states in thin-film monoclinic Ag₂Se. **2023**, 32, 101013 ○

- 480 Ferroelectricity and High Curie Temperature in a 2D Janus Magnet. ○
- 479 Positron trapping at the effective open volume in FeCr alloy containing hydrogen/helium atoms. **2023**, 9, 011001-011001 ○
- 478 High pseudocapacitive lithium-storage behaviors of amorphous titanium oxides with titanium vacancies and open channels. **2023**, 444, 142021 ○
- 477 Quantum Anomalous Hall Effects Controlled by Chiral Domain Walls. **2023**, 40, 037502 ○
- 476 Bubbles as a platform for investigating work function tunability of 2D materials under biaxial strains. **2023**, 60, 101978 ○
- 475 Tuning charge carrier dynamics through spacer cation functionalization in layered halide perovskites: an ab initio quantum dynamics study. **2023**, 11, 3521-3532 ○
- 474 Three-Dimensional Carbon Foam Modified with Mg₃N₂ for Ultralong Cyclability of a Dendrite-Free Li Metal Anode. ○
- 473 Tuning Catalytic Performance of C₂N/GaN Heterostructure for Hydrogen Evolution Reaction by Doping. **2023**, 6, ○
- 472 Ab Initio Study of Adsorption of Polymers on Metal-Organic Framework Surfaces. **2023**, 127, 3715-3725 ○
- 471 First-principles study on the thermoelectric properties of Sr₂Si and Sr₂Ge. **2023**, 32, 101015 ○
- 470 Surface Tamm States of 28 nm Nanodiamond via Raman Spectroscopy. **2023**, 13, 696 ○
- 469 Effects of hydrostatic pressure on the thermoelectric performance of BaZrS₃. **2023**, 138, ○
- 468 Pt : Ge Ratio as a Lever of Activity and Selectivity Control of Supported PtGe Clusters in Thermal Dehydrogenation**. **2023**, 15, ○
- 467 Different Doping of VSe₂ Monolayers as Adsorbent and Gas Sensing Material for Scavenging and Detecting SF₆ Decomposed Species. **2023**, 39, 2618-2630 1
- 466 Electrolyte effect for carbon dioxide reduction reaction on copper electrode interface: A DFT prediction. **2023**, 158, 094704 ○
- 465 An ab initio method on large sized molecular aggregate system: Predicting absorption spectra of crystalline organic semiconducting films. **2023**, 158, 094108 ○
- 464 First-Principles Density Functional Theory and Machine Learning Technique for the Prediction of Water Adsorption Site on PtPd-Based High-Entropy-Alloy Catalysts. **2023**, 6, ○
- 463 Single Atom Catalysis for Hydrogen Evolution Reaction using Transition-metal Atoms Doped g-C₃N₃: A Density Functional Theory Study. **2023**, 8, ○

- 462 Effect of substitution of 3d, 4d and 5d elements on structural, electronic, magnetic properties and XMCD spectra of Co-based full Heusler alloys: A DFT study. **2023**, 13, 025152 ○
- 461 Activation of CO₂ by Direct Cleavage Triggered by Photoelectrons on Rutile TiO₂(110). **2023**, 14, 1928-1933 ○
- 460 First-Principles Study of the Doping Effect in Half Delithiated LiNiO₂ Cathodes. **2023**, 6, 2134-2139 ○
- 459 Fermi-Level Instability as a Way to Tailor the Properties of La₃Te₄. **2023**, 14, 1962-1967 ○
- 458 Proton migration barriers in BaFeO₃ insights from DFT calculations. **2023**, 11, 6336-6348 ○
- 457 Unlocking the electronic, optical and transport properties of semiconductor coupled quantum dots using first principles methods. ○
- 456 pH- and Facet-Dependent Surface Chemistry of TiO₂ in Aqueous Environment from First Principles. **2023**, 15, 11216-11224 ○
- 455 Indirect Z-scheme hydrogen production photocatalyst based on two-dimensional GeC/MoSi₂N₄ van der Waals heterostructures. **2023**, ○
- 454 High-Pressure Pulsing of Ammonia Results in Carbamate as Strongly Inhibiting Adsorbate of Methanol Synthesis over Cu/ZnO/Al₂O₃. **2023**, 127, 3497-3505 ○
- 453 Suppressing Nonradiative Recombination by Electron-Donating Substituents in 2D Conjugated Triphenylamine Polymers toward Efficient Perovskite Optoelectronics. **2023**, 23, 1954-1960 ○
- 452 Catalytically Induced Robust Inorganic-Rich Cathode Electrolyte Interphase for 4.5 V Li||NCM622 Batteries. 2212150 3
- 451 Improving lithium polysulfides adsorption by oxygen-vacancy defects: By first-principles calculation. **2023**, 220, 112038 ○
- 450 Double-perovskite van der Waals heterostructure Cs₂NaInCl₆-XS₂ (X=Cr, Mo, W) as great potential material in photovoltaic devices. **2023**, 37, 102734 ○
- 449 First-principles study for discovery of novel synthesizable 2D high-entropy transition metal carbides (MXenes). **2023**, 11, 5681-5695 ○
- 448 A New Group of 2D Non-van der Waals Materials with Ultra Low Exfoliation Energies. **2023**, 9, ○
- 447 Strategies to Improve the Oxygen Reduction Reaction Activity on PtBi Bimetallic Catalysts: A Density Functional Theory Study. **2023**, 14, 1990-1998 ○
- 446 Tailoring alloy compositions by glucose towards superior Ni₂u₂ electrocatalysts for hydrogen evolution reaction. **2023**, ○
- 445 Hysteresis and training effect in the electric control of spin current in Pt/Y₃Fe₅O₁₂ heterostructures. **2023**, 107, ○

- 444 Non-Kitaev versus Kitaev honeycomb cobaltates. **2023**, 107, ○
- 443 Nanoscale-mixed ZnNiCu hydroxide composite catalyst for improved photocatalytic hydrogen evolution. **2023**, ○
- 442 Bottom-up building of two-dimensional magnetic materials with self-assembly of superatom TM@Sn₁₂ (TM = Sc, Ti, V, Cr, Mn, Fe) clusters. **2023**, 56, 144001 ○
- 441 Role of oxygen vacancies on surface reaction of water oxidation in WO₃ studied by density functional theory (DFT) and experiment. **2023**, 539, 113005 1
- 440 Structure-controlled valley splitting and anomalous valley Hall effect in Janus VSe₂/VSeX (X = S, Te) heterojunctions. **2023**, 56, 135301 ○
- 439 Uptake of Pb and the Formation of Mixed (Ba,Pb)SO₄ Monolayers on Barite During Cyclic Exposure to Lead-Containing Sulfuric Acid. **2023**, 15, 10593-10605 ○
- 438 Novel 2D sulfur-doped V₂O₅ flakes and their applications in photoelectrochemical water oxidation and high-performance energy storage supercapacitors. **2023**, 461, 141935 ○
- 437 Density functional theory-based quantum-computational analysis on the strain-assisted electronic and photocatalytic properties of BX-MSSe (X = P, As and M = Mo, W) heterostructures. **2023**, 129, ○
- 436 On the Nature of Hydrophobic Organic Compound Adsorption to Smectite Minerals Using the Example of Hexachlorobenzene-Montmorillonite Interactions. **2023**, 13, 280 ○
- 435 Effect of intrinsic point defects on the catalytic and electronic properties of Cu₂WS₄ single layer: Ab initio calculations. **2023**, 7, ○
- 434 Combining Machine Learning and Many-Body Calculations: Coverage-Dependent Adsorption of CO on Rh(111). **2023**, 130, ○
- 433 Lifting surface reconstruction of Au (100) by tellurium adsorption. ○
- 432 Identifying the ground state structures of point defects in solids. **2023**, 9, ○
- 431 Decoding Li + /Na + Exchange Route Toward High-Performance Mn-Based Layered Cathodes for Li-Ion Batteries. 2214921 ○
- 430 Why can cobalt(III) corrole form more stable metal/organic interfaces than cobalt(II) porphyrin?. A-L ○
- 429 Mechanical and electronic properties of transition metal hexa-nitrides in hexagonal structure from density functional theory calculations. **2023**, 221, 112084 ○
- 428 Synthesis, properties and catalytic performance of the novel, pseudo-spinel, multicomponent transition-metal selenides. **2023**, 11, 5337-5349 ○
- 427 Dual-Atom-Site Sn-Cu/C₃N₄ Photocatalyst Selectively Produces Formaldehyde from CO₂ Reduction. 2212453 ○

- 426 Reversible Luminescent Switching Induced by Heat/Water Treatment in a Zero-Dimensional Hybrid Antimony(III) Chloride. **2023**, 28, 1978 ○
- 425 Dynamic crystallography reveals spontaneous anisotropy in cubic GeTe. **2023**, 22, 311-315 1
- 424 Abnormal thermal expansion coefficients in $(\text{Nd}_{1-x}\text{Dy}_x)_2\text{Zr}_2\text{O}_7$ pyrochlore: The effect of low-lying optical phonons. **2023**, 1-14 ○
- 423 NaGaSe₂: A Water-Loving Multifunctional Non-van der Waals Layered Selenogallate. **2023**, 62, 3886-3895 ○
- 422 Evidences of Topological Surface States in the Nodal-Line Semimetal SnTaS₂ Nanoflakes. **2023**, 17, 4913-4921 ○
- 421 Unveiling a high capacity multi-redox (Nb⁵⁺/Nb⁴⁺/Nb³⁺) NASICON-Nb₂(PO₄)₃ anode for Li- and Na-ion batteries. **2023**, 11, 8173-8183 ○
- 420 Tuning the Mottness in Sr₃Ir₂O₇ via Bridging Oxygen Vacancies. **2023**, 40, 037101 ○
- 419 Molecular dynamics simulations of displacement cascades in vanadium: Generation and types of dislocation loops. **2023**, 34, 101394 ○
- 418 Electronic structure, magnetic properties, spin orientation, and doping effect in Mn₃Si₂Te₆. **2023**, 107, ○
- 417 First-principles theoretical analysis of magnetically tunable topological semimetallic states in antiferromagnetic DyPdBi. **2023**, 107, ○
- 416 Multiple Quantum States Induced in 1T-TaSe₂ by Controlling the Stacking Order of Charge Density Waves. 2214583 ○
- 415 Origin of contrasting trends of intrinsic electron mobility with tensile strain in hexagonal MoS₂ and triangular PdSe₂. **2023**, 107, ○
- 414 Antiferromagnetic topological magnetism in synthetic van der Waals antiferromagnets. **2023**, 107, ○
- 413 First-principles rationalization of self-reduction and lanthanide defect levels in SrB₄O₇. **2023**, 107, ○
- 412 Ion Kinetics and Capacity Tailoring in Stacked Graphdiyne by Functionalization. **2023**, 8, 8441-8447 ○
- 411 First principles study of the electronic structure of the Ni₂MnIn/InAs and Ti₂MnIn/InSb. **2023**, 7, ○
- 410 Determining surface-specific Hubbard-U corrections and identifying key adsorbates on nickel and cobalt oxide catalyst surfaces. **2023**, 25, 8903-8912 ○
- 409 Orthogonal luminescence lifetime encoding by intermetallic energy transfer in heterometallic rare-earth MOFs. **2023**, 14, ○

- 408 Single Ru(II) Ions on Ceria as a Highly Active Catalyst for Abatement of NO. **2023**, 145, 5029-5040 ○
- 407 Geometric frustration of Jahn-Teller order in the infinite-layer lattice. **2023**, 615, 237-243 ○
- 406 Comprehensive study on electronic structures of SiGe/Ga₂SeTe vdW heterobilayer. **2023**, 58, 4020-4030 ○
- 405 Hierarchically porous Ni foam-supported Co and Sn doped Ni₃S₂ nanosheets for oxygen evolution reaction electrocatalysts. **2023**, 11, 5734-5745 ○
- 404 Active sampling for neural network potentials: Accelerated simulations of shear-induced deformation in CuNi multilayers. **2023**, 158, 114103 ○
- 403 Remarkable plasticity and softness of polymorphic InSe van der Waals crystals. **2023**, ○
- 402 Structure-property relationship of reversible magnetic chirality tuning. **2023**, 107, ○
- 401 Large magnetoresistance and temperature-driven spin filter effect in spin valve based on half Heusler alloy. **2023**, 158, 114706 ○
- 400 Role of MoO_x/Ni(111) interfacial sites in direct deoxygenation of phenol toward benzene. **2023**, 13, 2201-2211 ○
- 399 ANi₅Bi_{5.6+} (A = K, Rb, and Cs): Quasi-One-Dimensional Metals Featuring [Ni₅Bi_{5.6+}] Double-Walled Column with Strong Diamagnetism. **2023**, 62, 3788-3798 ○
- 398 Toward Atomistic Understanding of Materials with the Conversion Alloying Mechanism in Li-Ion Batteries. **2023**, 35, 2835-2845 ○
- 397 Metal-decorated Graphyne as a drug transporting agent for the mercaptopurine chemotherapy drug: a DFT study. **2023**, 25, 9461-9471 ○
- 396 Strain-Induced Ferroelectric Phase Transition in Group-V Monolayer Black Phosphorus. **2023**, 6, ○
- 395 Thermodynamic stability of LiB₁₂ compounds from first principles. **2023**, 25, 7344-7353 ○
- 394 Diamane-like Films Based on Twisted G/BN Bilayers: DFT Modelling of Atomic Structures and Electronic Properties. **2023**, 13, 841 ○
- 393 High thermoelectric performance of layered LaAgXO (X=Se,Te) from electrical and thermal transport calculations. **2023**, 7, ○
- 392 Physical Insights on the Phonon Dispersion of TiS₂. 2200821 ○
- 391 Pseudo-Elasticity and Variable Electro-Conductivity Mediated by Size-Dependent Deformation Twinning in Molybdenum Nanocrystals. 2206380 ○

- 390 Theoretical investigation of the MXene precursors $\text{MoxV}_{4-x}\text{AlC}_3$ (0 \leq x \leq 4). **2023**, 13, ○
- 389 Effect of Co substitution on ferrimagnetic Heusler compound Mn_3Ga . **2023**, 49, 78-82 ○
- 388 Drastic oscillation of peierls stress from peierls-nabarro model calculation and its remedy. **2023**, 23, 5502-5519 ○
- 387 Hydrogen-Bond-Mediated Surface Functionalization of Boron Nitride Micro-Lamellae toward High Thermal Conductive Papers. **2023**, 10, ○
- 386 Mixed Microscopic Eu^{2+} Occupancies in the Next-Generation Red LED Phosphor $\text{Sr}[\text{Li}_2\text{Al}_2\text{O}_2\text{N}_2]_2\text{Eu}^{2+}$ (SALON:Eu²⁺). 2202732 ○
- 385 Tiny (ZnO) clusters supported on graphene for solar energy trapping: A density functional theory study. **2023**, 144, 104769 ○
- 384 Exploring the relationship between lattice distortion and phase stability in a multi-principal element alloy system based on machine learning method. **2023**, 221, 112089 ○
- 383 Analytical Forces for the Optimized Effective Potential Calculations. **2023**, 19, 1744-1752 ○
- 382 Tuning scintillation properties of Lu_2SiO_5 by Ce and Ca codoping. **2023**, 107, ○
- 381 Regulating Hollow Carbon Cage Supported NiCo Alloy Nanoparticles for Efficient Electrocatalytic Hydrogen Evolution Reaction. **2023**, 15, 12078-12087 ○
- 380 Density functional theory study of Br doped CsPbI_3 perovskite for photovoltaic and optoelectronic applications. **2023**, 98, 045505 ○
- 379 Understanding photoluminescence of bismuth-doped ternary alkaline earth d10 metal oxides via first-principles calculations. **2023**, 107, ○
- 378 Thermodynamics of diamond formation from hydrocarbon mixtures in planets. **2023**, 14, 1 ○
- 377 Achieving Ultra-High Selectivity to Hydrogen Production from Formic Acid on PdAg Alloys. **2023**, 145, 5114-5124 ○
- 376 Structural properties of Bi/Au(110). **2023**, 34, 235601 ○
- 375 The Atomistic Understanding of the Ice Recrystallization Inhibition Activity of Antifreeze Glycoproteins. **2023**, 13, 405 ○
- 374 Electrical and thermal conductivity of fcc and hcp iron under conditions of the Earth's core from ab initio simulations. **2023**, 107, 1
- 373 Room-temperature photosynthesis of propane from CO_2 with Cu single atoms on vacancy-rich TiO_2 . **2023**, 14, ○

- 372 Theoretical analysis of electrochromism of Ni-deficient nickel oxide [From bulk to surfaces]. **2023**, 25, 7974-7985 ○
- 371 Catalytic CO Oxidation by Single Atom Catalysts of Transition Metal-doped β -Borophene: A First Principles Study. **2023**, 52, 249-253 ○
- 370 Strain effect on the high T_c superconductor $\text{YBa}_2\text{Cu}_3\text{O}_7$: an ab initio study comparing bulk and monolayer models. **2023**, 5, 015002 ○
- 369 Extended calculation of electronic excitations for direct detection of dark matter. **2023**, 107, ○
- 368 Comprehensive Mechanism for CO Electroreduction on Dual-Atom-Catalyst-Anchored N-Doped Graphene. ○
- 367 Geometric Tuning of Single-Atom FeN₄ Sites via Edge-Generation Enhances Multi-Enzymatic Properties. ○
- 366 Machine Learning Molecular Dynamics Simulations for Evaluation of High-Temperature Properties of Nuclear Fuel Materials. **2023**, 62, 175-181 ○
- 365 Stacking-dependent topological magnons in bilayer CrI_3 . **2023**, 7, ○
- 364 An Efficient Way to Model Complex Iron Carbides: A Benchmark Study of DFTB2 against DFT. **2023**, 127, 2071-2080 1
- 363 Amorphous As_2S_3 Doped with Transition Metals: An Ab Initio Study of Electronic Structure and Magnetic Properties. **2023**, 13, 896 ○
- 362 Electric-Field Emission Mechanism in Q-Carbon Field Emitters. **2023**, 8, 9307-9318 ○
- 361 Designing polar textures with ultrafast neuromorphic features from atomistic simulations. **2023**, 3, 012002 ○
- 360 The single-atom catalytic activity of the hydrogen evolution reaction of the experimentally synthesized boridene 2D material: a density functional theory study. **2023**, 29, ○
- 359 Topological Nodal Surface and Quadratic Dirac Semimetal States and van Hove Singularities in ScH_3 and LuH_3 Superconductors. **2023**, 8, 9607-9613 ○
- 358 The Microzone Structure Regulation of Diamond/Cu-B Composites for High Thermal Conductivity: Combining Experiments and First-Principles Calculations. **2023**, 16, 2021 ○
- 357 Theoretical Evaluation of Highly Efficient Nitrate Reduction to Ammonia on InBi . **2023**, 14, 2410-2415 ○
- 356 Analysis of diffuse scattering in electron diffraction data for the crystal structure determination of Pigment Orange 13, $\text{C}_{32}\text{H}_{24}\text{Cl}_2\text{N}_8\text{O}_2$. **2023**, 79, 122-137 ○
- 355 Dzyaloshinskii-Moriya interaction and skyrmions in antiferromagnetic-based heterostructures. **2023**, 572, 170594 ○

- 354 Revisiting the Storage Capacity Limit of Graphite Battery Anodes: Spontaneous Lithium Overintercalation at Ambient Pressure. **2023**, 2, ○
- 353 Construction of Localized High-Concentration PF₆⁻ Region for Suppressing NCM622 Cathode Failure at High Voltage. 2201693 ○
- 352 Anharmonic phonon renormalization and two-channel thermal transport in SrTiO₃ using full temperature-dependent interatomic force constant. **2023**, 467, 128727 ○
- 351 Ti-6Al-4V to over 1.2 TPa: Shock Hugoniot experiments, ab initio calculations, and a broad-range multiphase equation of state. **2023**, 107, ○
- 350 Origin of superconductivity in hole doped SrBiO₃ bismuth oxide perovskite from parameter-free first-principles simulations. **2023**, 9, ○
- 349 Influence of Nitrogen Substitution on the Electronic Structure of Ti₂O₃: Insights into the Doping-Induced Insulator-to-Metal Transition. 2200495 ○
- 348 Spinel-Anchored Iridium Single Atoms Enable Efficient Acidic Water Oxidation via Intermediate Stabilization Effect. **2023**, 13, 3757-3767 ○
- 347 Oxygen Vacancy Promoted Generation of Monatomic Oxygen Anion over Ni²⁺-Doped MgO for Efficient Glycolysis of Waste PET**. ○
- 346 Morphology-controlled Co_{0.5}Ni_{0.5}S₂-C double-shell porous microspheres for the construction of high-performance asymmetric supercapacitors. **2023**, 447, 142149 ○
- 345 Electromagnetic evolution in proton-containing spinel NiCo₂O₄ thin films via ionic liquid gating. **2023**, 107, ○
- 344 Polysulfide cluster formation, surface reaction, and role of fluorinated additive on solid electrolyte interphase formation at sodium-metal anode for sodium-sulfur batteries. **2023**, 158, 124706 ○
- 343 Lithium Ion Transport Environment by Molecular Vibrations in Ion-Conducting Glasses. ○
- 342 Nanoscale Chemical Heterogeneity Ensures Unprecedentedly Low Resistance Drift in Cache-Type Phase-Change Memory Materials. **2023**, 23, 2362-2369 ○
- 341 Interface and energy band manipulation of Bi₂O₃-Bi₂S₃ electrode enabling advanced magnesium-ion storage. **2023**, ○
- 340 Efficient Inorganic Vapor-Assisted Defects Passivation for Perovskite Solar Module. ○
- 339 Crystal-chemical characterization and spectroscopy of fluorcarletonite and carletonite. 1-28 ○
- 338 Directing and Understanding the Translation of a Single Molecule Dipole. **2023**, 14, 2487-2492 ○
- 337 Computational and experimental investigations on the effect of crystallinity and crystal size on Na-transport in nanoscaled Si: implications for Si-based anodes for Na-ion batteries. **2023**, 27, 1227-1240 ○

- 336 Achieving superb strength in single-phase FCC alloys via maximizing volume misfit. **2023**, 63, 108-119 1
- 335 Lab-on-Fiber Based on Optimized Gallium Selenide for Femtosecond Mode-Locked Lasers and Fiber-Compatible Photodetectors. **2023**, 4, 0
- 334 Upcycling natural Limestone waste for thermochemical energy storage by utilising tailored CaZrO₃ nanoadditives. 0
- 333 Theoretical study on the magnetic properties of cathode materials in the lithium-ion battery. **2023**, 158, 124702 0
- 332 Surface-Dependent Electrocatalytic Activity of CoSe₂ for Lithium Sulfur Battery. **2023**, 10, 0
- 331 Electronic structural and lattice thermodynamic properties of MAO₂ and M₅AlO₄ (M = Li, Na, K) sorbents for CO₂ capture applications. **2023**, 3, 0
- 330 Enabling an Intrinsically Safe and High-Energy-Density 4.5 V-Class Lithium-Ion Battery with Synergistically Incorporated Fast Ion Conductors. 2203999 0
- 329 Effect of bromide incorporation on the electronic & photovoltaic properties of Sn-based perovskite devices: A multiscale investigation utilizing first principles approach and numerical simulation, aided by machine learning models. **2023**, 253, 375-388 0
- 328 Regulating the Unhybridized O 2 p Orbitals of High-Performance Li-Rich Mn-Based Layered Oxide Cathode by Gd-Doping Induced Bulk Oxygen Vacancies. 2214613 0
- 327 Photoinduced Dynamics at the Water/TiO₂(101) Interface. **2023**, 130, 0
- 326 Gold Nanoparticles Enriched Graphene System for Therapeutics: A Novel Combination of Experimental and Theoretical Studies. 0
- 325 Revealing the promising near-room-temperature thermoelectric performance in Ag₂Se single crystals. **2023**, 0
- 324 Methane Activation and Coupling Pathways on Ni₂P Catalyst. **2023**, 13, 531 0
- 323 Twisted Crystalline Organic Semiconductor Photodetectors. 2212531 0
- 322 Effect of the surface termination on the adsorption of flue gas by the titanium carbide MXene. **2023**, 29, 101441 0
- 321 Aromatic hexazine [N₆]⁴⁻ anion featured in the complex structure of the high-pressure potassium nitrogen compound K₉N₅6. 0
- 320 The enhanced photocatalytic and photothermal effects of Ti₃C₂ MXene quantum dot/macroscale porous graphitic carbon nitride heterojunction for Hydrogen Production. **2023**, 641, 309-318 0
- 319 Exploring the Structural and Elastic Properties of CH₃NH₃Gel₃ under High Pressure Based on First Principle Calculations. 0

- 318 First-Principles Modeling of the Adsorption Mechanism of Carboxylic and Phosphonic Acids onto Pristine and Defective Delafossite CuAlO₂ Surfaces. 0
- 317 No magma ocean surface after giant impacts between rocky planets. **2023**, 608, 118014 1
- 316 Electrically tunable Gilbert damping in van der Waals heterostructures of two-dimensional ferromagnetic metals and ferroelectrics. **2023**, 122, 102402 0
- 315 Development of Deep Potentials of Molten MgCl₂/NaCl and MgCl₂/KCl Salts Driven by Machine Learning. 0
- 314 Anharmonic phonon behavior via irreducible derivatives: Self-consistent perturbation theory and molecular dynamics. **2023**, 107, 0
- 313 The versatile characteristics of ArS/SGaInS van der Waals heterostructures. 0
- 312 High reactivity of mesoporous CeO₂ to dissociate chemical warfare agent sarin. 0
- 311 Comparative studies of hexagonal boron phosphide/V₂CS₂ heterostructure and homogeneous bilayers as metal-ion battery anodes. **2023**, 25, 10011-10021 0
- 310 A Priori Design of Dual-Atom Alloy Sites and Experimental Demonstration of Ethanol Dehydrogenation and Dehydration on PtCrAg. 0
- 309 (n, m) Distribution of Single-Walled Carbon Nanotubes Grown from a Non-Magnetic Palladium Catalyst. **2023**, 28, 2453 0
- 308 Computational studies on functionalized Janus MXenes MM₂CT₂, (M, M₂ = Zr, Ti, Hf, M₂ ≠ M; T = D, E, OH): photoelectronic properties and potential photocatalytic activities. **2023**, 13, 7972-7979 0
- 307 Coupling interface constructions of FeOOH/NiCo₂S₄ by microwave-assisted method for efficient oxygen evolution reaction. 0
- 306 Water Oxidation-Induced Surface Reconstruction and Dissolution at the RuO₂(110) Surface Revealed by First-Principles Simulation. **2023**, 127, 5334-5342 0
- 305 Coexistence and coupling of ferroelectricity and magnetism in an oxide two-dimensional electron gas. 0
- 304 Asymmetric Janus functionalization induced magnetization and switchable out-of-plane polarization in 2D MXene Mo₂CXX₂. **2023**, 25, 8676-8683 0
- 303 A two-dimensional tetragonal structure of vanadium telluride. 0
- 302 Investigation of Rechargeable Calcium Metal-Selenium Batteries Enabled by Borate-Based Electrolytes. **2023**, 35, 2363-2370 0
- 301 Copper Cobalt Selenide as a Bifunctional Electrocatalyst for the Selective Reduction of CO₂ to Carbon-Rich Products and Alcohol Oxidation. 0

- 300 Theoretical exploration on the activity of copper single-atom catalysts for electrocatalytic reduction of CO₂. **2023**, 11, 7735-7745 ○
- 299 Engineering the catalytic properties of CeO₂ catalyst in HCl-assisted propane dehydrogenation by effective doping: A first-principles-based microkinetic simulation. 11, ○
- 298 Two-Dimensional Iron Silicide (FeSi₂) Alloys with Above-Room-Temperature Ferromagnetism. **2023**, 23, 2332-2338 ○
- 297 BSSE-corrected consistent Gaussian basis sets of triple-zeta valence quality of the lanthanides La-Lu for solid-state calculations. ○
- 296 Electrochemical Reduction of Nitrates on CoO Nanoclusters-Functionalized Graphene with Highest Mass Activity and Nearly 100% Selectivity to Ammonia. 2204236 ○
- 295 Interface synergism and engineering of Pd/Co@N-C for direct ethanol fuel cells. **2023**, 14, ○
- 294 From high-entropy alloys to high-entropy ceramics: The radiation-resistant highly concentrated refractory carbide (CrNbTaTiW)₄C. **2023**, 250, 118856 ○
- 293 Theoretical investigation of charge transfer between two defects in a wide band gap semiconductor. **2023**, 107, ○
- 292 Decreased spin-resolved anti-bonding states filling to accelerate CHO conversion into CH₂O in transitional metal-doped Mo₂C monolayers during CO₂ reduction. ○
- 291 Search for semiconducting materials among 18-electron half-Heusler alloys. **2023**, 364, 115133 ○
- 290 Massively parallel GPU enabled third-order cluster perturbation excitation energies for cost-effective large scale excitation energy calculations. **2023**, 158, 144111 ○
- 289 Neural network potentials for accelerated metadynamics of oxygen reduction kinetics at Au/water interfaces. **2023**, 14, 3913-3922 ○
- 288 Mechanisms of adsorbing hydrogen gas on metal decorated graphene. **2023**, 7, ○
- 287 Computational Modelling of Pyrrolic MN₄ Motifs Embedded in Graphene for Catalyst Design. **2023**, 13, 566 ○
- 286 Importance of Adatom on Pure Iron Catalyst Towards Electrocatalytic N₂ Reduction Reaction. ○
- 285 Hydration Mechanisms of Tungsten Trioxide Revealed by Water Adsorption Isotherms and First-Principles Molecular Dynamics Simulations. **2023**, 127, 5584-5596 ○
- 284 Direct Atomic-Level Insight into Oxygen Reduction Reaction on Size-Dependent Pt-based Electrocatalysts from Density Functional Theory Calculations. **2023**, ○
- 283 Topological band inversion in HgTe(001): Surface and bulk signatures from photoemission. **2023**, 107, ○

- 282 Quantum Catalytic Performance for the Hydrogen Evolution Reaction and the Ethanol Oxidation Reaction in Topological Edge States of SrPd and BaPd Semimetal Monolayers: A Theoretical Study. **2023**, 127, 5271-5280 ○
- 281 First-Principles Study of Group VA Monolayer Passivators for Perovskite Solar Cells. **2023**, 6, 4279-4287 ○
- 280 Probing Local Environments of Oxygen Vacancies Responsible for Hydration in Sc-Doped Barium Zirconates at Elevated Temperatures: In Situ X-ray Absorption Spectroscopy, Thermogravimetry, and Active Learning Ab Initio Replica Exchange Monte Carlo Simulations. **2023**, 35, 2289-2301 ○
- 279 Structural Reconstruction Modulated Physical Properties of Titanium Oxide at the Monolayer Limit. **2023**, 127, 5631-5639 ○
- 278 Magnetic proximity effect in LaO/EuO heterostructures: A first-principles study. **2023**, 107, ○
- 277 Electrical conductivity of iron in Earth's core from microscopic Ohm's law. **2023**, 107, 1
- 276 The recent progress of laser-induced graphene based device applications. **2023**, 44, 031701 ○
- 275 Band alignment at the strontium germanate interface with silicon. **2023**, 107, ○
- 274 Synthesis and Characterization of the Orthorhombic Sn₃O₄ Polymorph. **2023**, 135, ○
- 273 Insights into Active Sites and Mechanisms of Benzyl Alcohol Oxidation on Nickel/Iron Oxyhydroxide Electrodes. **2023**, 13, 4272-4282 ○
- 272 Synthesis and Characterization of the Orthorhombic Sn₃O₄ Polymorph. **2023**, 62, ○
- 271 Mechanistic Insights into Nonoxidative Ethanol Dehydrogenation on NiCu Single-Atom Alloys. **2023**, 13, 4290-4303 ○
- 270 Mechanistic origins of accelerated hydrogenation of mixed alkylaromatics by synchronised adsorption over Rh/SiO₂. ○
- 269 Sustainable methane utilization technology via photocatalytic halogenation with alkali halides. **2023**, 14, ○
- 268 Computational Design and Theoretical Properties of WC₃N₆, an H-Free Melaminite and Potential Multifunctional Material. **2023**, 145, 6986-6993 ○
- 267 Selective Photochromic Response to Low-Dose X-ray Radiation Detection in One-Dimensional Cadmium-Viologen Complexes. **2023**, 62, 4990-4998 ○
- 266 Predicting thermoelectric transport properties from composition with attention-based deep learning. **2023**, 4, 015037 ○
- 265 Methanol Synthesis on Copper-Doped F Centers. **2023**, 127, 5321-5333 ○

- 264 Study of pnictides for photovoltaic applications. **2023**, 25, 9626-9635 ○
- 263 Atomically Sharp Internal Interface in a Chiral Weyl Semimetal Nanowire. **2023**, 23, 2695-2702 ○
- 262 First-Principles Study on Thermoelectric Properties of Bi₂Se₃. ○
- 261 Hot carrier relaxation dynamics in non-stoichiometric CdSe quantum dots: computational insights. **2023**, 11, 8256-8264 ○
- 260 Intercalation of p-Aminopyridine and p-Ethylenediamine Molecules into Orthorhombic In_{1.2}Ga_{0.8}S₃ Single Crystals. **2023**, 16, 2368 ○
- 259 Multifunctional Coatings on Sulfide-Based Solid Electrolyte Powders with Enhanced Processability, Stability, and Performance for Solid-State Batteries. ○
- 258 Novel tungsten nitride crystal providing nanochannels for hydrogen removal and recycling in PFMs. **2023**, 158, 124125 ○
- 257 New Insights on the Tensile Strength and Fracture Mechanism of c-ZrO₂/m-Al₂O₃ Interfaces. **2023**, 13, 3742 ○
- 256 Ferroelectric and negative piezoelectric properties in oxyhydroxide monolayers XOOH (X = Al, Ga, and In). ○
- 255 First-Principles and Experimental Study of Trace Impurities and Near-Infrared Emission in Alkaline Earth Hexaaluminates. **2023**, 35, 2999-3007 ○
- 254 Phase transition, optical, and elastic properties of a new hybrid organic-inorganic perovskite: [(R)-(+)-3-aminoquinuclidine]Kl₃. **2023**, 11, 031110 ○
- 253 Quantum paraelectricity and structural phase transitions in strontium titanate beyond density functional theory. **2023**, 7, ○
- 252 Lattice dynamics and in-plane antiferromagnetism in Mn_xZn_{1-x}PS₃ across the entire composition range. **2023**, 107, ○
- 251 Critical interphase overpotential as a lithium dendrite-suppression criterion for all-solid-state lithium battery design. ○
- 250 Spin-phonon interaction and short-range order in Mn₃Si₂Te₆. **2023**, 107, ○
- 249 Absorption Modulation and Anomalous Thermal Transport in Two-dimensional X-AlN (X=C, Si, TC) Semiconductor. **2023**, 0 ○
- 248 Effect of Adsorbed Sulfate on the Product Selectivity of Ethanol Oxidation on Pt Nanoparticles in Acidic Solution. **2023**, 127, 5743-5753 ○
- 247 Iron and nitrogen co-modified multi-walled carbon nanotubes for efficient electrocatalytic oxygen reduction. **2023**, 34, 245403 ○

- 246 Frequency Splitting of Chiral Phonons from Broken Time-Reversal Symmetry in CrI₃. **2023**, 130, ○
- 245 Antiferromagnetic FeTe₂ 1T \bar{C} phase formation at the Sb₂Te₃. **2023**, 7, ○
- 244 Water adsorption on lead dioxide from ab initio molecular dynamics simulations. **2023**, 158, 134718 ○
- 243 Semimetal contacts to monolayer semiconductor: weak metalization as an effective mechanism to Schottky barrier lowering. **2023**, 56, 234001 ○
- 242 The effects of point defects on thermal-mechanical properties of BiCuOTe: a first-principles study. **2023**, 25, 10715-10725 ○
- 241 Approaching the free-ion limit in magnetically isotropic gadolinium(III) via borohydride ligands. **2023**, 25, 10689-10696 ○
- 240 Influence of Capping Ligands, Solvent, and Thermal Effects on CdSe Quantum Dot Optical Properties by DFT Calculations. **2023**, 8, 11467-11478 ○
- 239 Identification of Hydrogen Trapping in Aluminum Alloys Via Muon Spin Relaxation Method and First-Principles Calculations. ○
- 238 Orbital distortion and electric field control of sliding ferroelectricity in a boron nitride bilayer. **2023**, 35, 235001 ○
- 237 Thermoelastic Properties of Liquid Fe-Rich Alloys Under Martian Core Conditions. **2023**, 50, ○
- 236 RKKY interactions mediated by topological states in transition metal doped bismuthene. **2023**, 133, 115105 ○
- 235 Unfolding the structure-property relationships of Li₂S anchoring on two-dimensional materials with high-throughput calculations and machine learning. **2023**, 82, 31-39 ○
- 234 2D MoSi₂N₄ as electrode material of Li-air battery: A DFT study. **2023**, 25, ○
- 233 Activating bulk nickel foam for the electrochemical oxidization of ethanol by anchoring MnO₂@Au nanorods. **2023**, 11, 8101-8109 ○
- 232 Inhibition Mechanism of MgO Addition on High-Temperature Oxidation of Magnetite: Density Functional Theory and Ab Initio Molecular Dynamics Methods Joint Research and Experimental Verification. ○
- 231 Regulating the Coordination Environment of Single-Atom Catalysts Anchored on Thiophene Linked Porphyrin for an Efficient Nitrogen Reduction Reaction. **2023**, 15, 15545-15560 ○
- 230 Tailoring high-energy storage NaNbO₃-based materials from antiferroelectric to relaxor states. **2023**, 14, ○
- 229 Selective Oxidation of CH₄ to CH₃OH by Transition-Metal Single-Atom-Embedded N-Doped Graphene Catalysts with Oxidants N₂O and O₂: Oxygen Adsorption Energy as an Activity Descriptor. **2023**, 127, 5800-5809 ○

- 228 Theoretical study of the tuning role of β -methylthio or β -methylselenyl on the charge-transport properties of acenedithiophenes derivatives. **2023**, 25, 10313-10324 ○
- 227 Brønsted Acid Strength Does Not Change for Bulk and External Sites of MFI Except for Al Substitution Where Silanol Groups Form. **2023**, 13, 4470-4487 ○
- 226 The Role of Arsenic in the Operation of Electrical Threshold Switches. ○
- 225 Outstanding visible light photocatalysis using nano-TiO₂ hybrids with nitrogen-doped carbon quantum dots and/or reduced graphene oxide. ○
- 224 First-Principles Assessment of CdTe as a Tunnel Barrier at the β -Sn/InSb Interface. **2023**, 15, 16288-16298 ○
- 223 Theoretical study of the catalytic performance of Fe and Cu single-atom catalysts supported on Mo₂C toward the reverse water-gas shift reaction. 11, ○
- 222 Selective Interstitial Hydration Explains Anomalous Structural Distortions and Ionic Conductivity in 6H-Ba₄Ta₂O₉·1/2H₂O. **2023**, 35, 2740-2751 ○
- 221 Aromatic Clusters and Hydrogen Storage. **2023**, 16, 2833 ○
- 220 Engineering Catalytically Active Sites by Sculpting Artificial Edges on MoS₂ Basal Plane for Dinitrogen Reduction at a Low Overpotential. 2206357 ○
- 219 Strong Magnetocaloric Coupling in Oxyorthosilicate with Dense Gd³⁺ Spins. **2023**, 62, 5282-5291 ○
- 218 A DFT Study of Ruthenium fcc Nano-Dots: Size-Dependent Induced Magnetic Moments. **2023**, 13, 1118 ○
- 217 Improved Electrochemical Performance of Spinel LiNi_{0.5}Mn_{1.5}O₄ Cathode Materials with a Dual Structure Triggered by LiF at Low Calcination Temperature. **2023**, 15, 16778-16793 ○
- 216 First-principles study of square chalcogen bond interactions and its adsorption behavior on silver surface. **2023**, 25, 10836-10844 ○
- 215 Water Splitting on a Pt₁/C₃N₄ Single Atom Catalyst: A Modeling Approach. ○
- 214 Atomistic mechanisms for catalytic transformations of NO to NH₃, N₂O, and N₂ by Pd. **2023**, 36, 94-102 ○
- 213 Thermodynamics of phase stability and disorder in Inter-Lanthanide ternary ABO₃ oxides from first principles. **2023**, 228, 111830 ○
- 212 Intrinsic ferroelectrics and carrier doping-induced metallic multiferroics in an atomic wire. **2023**, ○
- 211 Experimental and theoretical thermodynamic studies in Ba₂MgReO₆ the ground state in the context of Jahn-Teller effect. **2023**, 35, 245603 ○

- 210 Crystal structures of two phases of Pigment Yellow 110 from X-ray powder diffraction data. **2023**, ○
- 209 Structural Bistability in RbI Monolayers on Ag(111). **2023**, 14, 3023-3030 ○
- 208 Effect of Linker Structure and Functionalization on Secondary Gas Formation in Metal-Organic Frameworks. **2023**, 127, 2881-2888 ○
- 207 Theoretical screening of single atom doping on β -Ga₂O₃ (100) for photoelectrochemical water splitting with high activity and low limiting potential. **2023**, 15, 6913-6919 ○
- 206 Transition-Metal-Free, Pure p-Block Alloy Electrocatalysts for the Highly Efficient Nitrate Reduction to Ammonia. **2023**, 35, 2884-2891 ○
- 205 Selective Self-Assembly and Modification of Herringbone Reconstructions at a Solid-Liquid Interface of Au(111). **2023**, 14, 3057-3062 ○
- 204 Geometrical and Electronic Structure Analysis of Mn-Doped CaMO₃ (M = Ti, Zr, and Sn). ○
- 203 First-principles study of the initial stage of Pentacene adsorption on the twofold surface of the Ag-In-Yb quasicrystal. **2023**, 2461, 012016 ○
- 202 Structure and Stability of Metalloporphyrin Networks on Au(111). **2023**, 127, 6569-6577 ○
- 201 First-Principle Calculations to Investigate the Elastic, Thermoelectric, and Electronic Performances of XRhSn (X = V, Nb, Ta) Half-Heusler Compounds. ○
- 200 Temperature dependence of magnetic anisotropy and magnetoelasticity from classical spin-lattice calculations. **2023**, 107, ○
- 199 Improving the creation of SiV centers in diamond via sub- μ s pulsed annealing treatment. ○
- 198 Advances in bismuth-telluride-based thermoelectric devices: progress and challenges. **2023**, 100122 ○
- 197 First principle study on transition metal ammine borohydrides with amphoteric hydrogen for hydrogen storage applications. **2023**, ○
- 196 Chemical Adsorption of HF, HCl, and H₂O onto YF₃ and Isostructural HoF₃ Surfaces by First Principles. **2023**, 13, 555 ○
- 195 DFT Calculation of High-Angle Kink Boundary in 18R-LPSO Alloy. **2023**, 64, 813-816 ○
- 194 Promising transition metal decorated borophene catalyst for water splitting. **2023**, 13, 9678-9685 ○
- 193 Size Limiting Elemental Ferroelectricity in Bi Nanoribbons: Observation, Mechanism, and Opportunity. **2023**, 14, 3160-3167 ○

- 192 Site-Selective Atomic Layer Deposition at Thermally Generated Surface Oxygen Vacancies on Rutile TiO₂. **2023**, 35, 2857-2863 ○
- 191 Electronic and strain-elimination effects of solute-vacancy interaction in molybdenum. **2023**, 133, 125106 ○
- 190 Large 3D anisotropy of magnetoresistance in MoAlB. **2023**, 33, 101060 ○
- 189 Enhancing efficiency of the ternary tri-chalcogenide MnPSe₃ towards hydrogen evolution reaction by activating its basal plane. **2023**, ○
- 188 Na⁺ Migration Mediated Phase Transitions Induced by Electric Field in the Framework Structured Tungsten Bronze. **2023**, 14, 3152-3159 ○
- 187 Multiplicity of Zn coordination sites at cubic spinel ferrites: magnetism and influence of the Zn d band. **2023**, 58, 5658-5677 ○
- 186 Modulation of oxygen-etching for generating nickel single atoms for efficient electroreduction of CO₂ to syngas (CO/H₂). **2023**, 421, 332-341 ○
- 185 Role of molecular modelling in the development of metal-organic framework for gas adsorption applications. **2023**, 135, ○
- 184 The importance of the image forces and dielectric environment in modeling contacts to two-dimensional materials. **2023**, 7, ○
- 183 Interface-vacancy synergy of Co(OH)₂/CoN to boost alkaline water splitting. ○
- 182 Unveiling the local structure of the amorphous metal $\text{Fe}_{1-x}\text{Zr}_x$ combining first-principles-based simulations and modelling of EXAFS spectra. **2023**, 13, ○
- 181 Molecular engineering of naphthalene spacers in low-dimensional perovskites. **2023**, 11, 5024-5031 ○
- 180 Deterministic Magnetic Switching in Perpendicular Magnetic Trilayers Through Sunlight-Induced Photoelectron Injection. ○
- 179 Nitrogen adsorption via charge transfer on vacancies created during surfactant assisted exfoliation of TiB₂. ○
- 178 Ab Initio Prediction of Ultra-Wide Band Gap B x Al 1x N Materials. ○
- 177 Factors controlling heteroepitaxial phase formation at intermetallic-Al₃Sc/liquid interfaces. **2023**, 133, 124902 ○
- 176 Role of Oxygen in Vacancy-Induced Phase Formation and Crystallization of Al₂TiO₅-Based Chemical Vapor-Deposited Coatings. **2023**, 127, 6456-6465 ○
- 175 Medium-Range Ordering in the Ionic Glass Electrolytes LiPON and LiSiPON. **2023**, 35, 2730-2739 ○

- 174 Predicting the Na⁺ ion transport properties of NaSICON materials using density functional theory and Kinetic Monte Carlo. ○
- 173 Binary molten salt in situ synthesis of sandwich-structure hybrids of hollow μ Mo₂C nanotubes and N-doped carbon nanosheets for hydrogen evolution reaction. ○
- 172 Defect engineering of silicon with ion pulses from laser acceleration. **2023**, 4, ○
- 171 Pressure-induced electride phase formation in calcium: A key to its strange high-pressure behavior. **2023**, 107, ○
- 170 Electrochemical partial reduction of Ni(OH)₂ to Ni(OH)₂/Ni via coupled oxidation of an interfacing NiAl intermetallic compound for robust hydrogen evolution. **2023**, ○
- 169 Unique (100) Surface Configuration Enables Promising Oxygen Reduction Performance for Pt₃Co Nanodendrite Catalysts. **2023**, 15, 18217-18228 ○
- 168 Field-tunable Weyl points and large anomalous Hall effect in the degenerate magnetic semiconductor EuMg₂Bi₂. **2023**, 107, ○
- 167 Silicate Dissolution Mechanism from Metakaolinite Using Density Functional Theory. **2023**, 13, 1196 ○
- 166 Dirac Points in Two-Dimensional Semi-Metal B5ScNi Monolayer with Low Symmetry. ○
- 165 Machine-learning accelerated annealing with fitting-search style for multicomponent alloy structure predictions. **2023**, 7, ○
- 164 Atomic scale interfacial magnetism and origin of metal-insulator transition in (LaNiO₃)_n/(CaMnO₃)_m superlattices: a first principles study. **2023**, 13, ○
- 163 Band Modification and Localized Lattice Engineering Leads to High Thermoelectric Performance in Ge and Bi Codoped SnTeAgBiTe₂ Alloys. ○
- 162 Highly Selective N₂ Electroreduction to NH₃ Using a Boron-Vacancy-Rich Diatomic Nb₂B Catalyst. ○
- 161 Experimental and Theoretical Investigations of Out-of-Plane Ordered Nanolaminate Transition Metal Borides: M₄CrSiB₂ (M = Mo, W, Nb). **2023**, 62, 5341-5347 ○
- 160 Towards quantum corrosion chemistry: screening perfect Cr, Ni sites and stoichiometry on top of an Fe(110) surface using DFT. **2023**, 13, 9945-9953 ○
- 159 First-principles investigation on the structural, vibrational, mechanical, electronic, and optical properties of MSi₂Z₄ (M : Pd and Pt, . **2023**, 7, ○
- 158 Polarizable Anionic Sublattices Can Screen Molecular Dipoles in Noncentrosymmetric Inorganic/Organic Hybrids. **2023**, 15, 18006-18011 ○
- 157 Real-time insight into the multistage mechanism of nanoparticle exsolution from a perovskite host surface. **2023**, 14, ○

- 156 In-plane momentum-dependent spin texture originating from surface symmetry breaking in the two-dimensional van der Waals ferromagnet CrGeTe₃. **2023**, 107, ○
- 155 Plasmons in a two-dimensional nonsymmorphic nodal-line semimetal. **2023**, 107, ○
- 154 Fast general two- and three-body interatomic potential. **2023**, 107, ○
- 153 Revisiting the Low-Index Surfaces of LaCoO₃ with a Passivation Strategy. **2023**, 127, 6843-6851 ○
- 152 Controlled Vertical Transfer of Individual Au Atoms Using a Surface Supported Carbon Radical for Atomically Precise Manufacturing. ○
- 151 Role of Chemical Etching in the Nucleation of Nanopores in 2D MoS₂: Insights from First-Principles Calculations. **2023**, 127, 6873-6883 ○
- 150 Spontaneous hydrogen production using gadolinium telluride. **2023**, 26, 106510 ○
- 149 Influences of C, Si and Mn on the wear resistance of coiled tubing steel. **2023**, 204854 ○
- 148 Polaron-induced metal-to-insulator transition in vanadium oxides from density functional theory calculations. **2023**, 107, ○
- 147 High-throughput screening of highly efficient Cu-based dual-atom catalysts to promote nitrate electroreduction for ammonia synthesis: A computational study. **2023**, 541, 113095 ○
- 146 On the Donor: Acceptor Features for Poly(3-hexylthiophene): TiO₂ Quantum Dots Hybrid Materials Obtained via Water Vapor Flow Assisted Sol-Gel Growth. **2023**, 15, 1706 ○
- 145 NbC. **2023**, 109, 323-332 ○
- 144 Metavalent Bonding in Layered Phase-Change Memory Materials. ○
- 143 Vanadium-Containing Planar Heterostructures Based on Topological Insulators. **2023**, 117, 228-233 ○
- 142 Experimental and Ab-Initio Investigation of the Electrical Conductivity of Emeraldine Salt. **2023**, 127, 6813-6824 ○
- 141 Intermetallic alloy structure-activity descriptors derived from inelastic X-ray scattering. ○
- 140 Lu₂Ni₃ Phase Diagram from First-Principles Calculations. **2023**, 40, 057401 ○
- 139 Improved Carrier Lifetimes of CdSe Thin Film via Te Doping for Photovoltaic Application. **2023**, 15, 17858-17866 ○

- 138 Impact of quartic anharmonicity on lattice thermal transport in EuTiO₃: a comparative theoretical and experimental investigation. **2023**, 101059 ○
- 137 Large electrical strain in lead-free K_{0.5}Na_{0.5}NbO₃-based ceramics by heterovalent doping. **2023**, ○
- 136 Solubility and diffusivity of hydrogen and its isotopes in the BeO system. ○
- 135 Theoretical Prediction of the Sublimation Behavior by Combining Ab Initio Calculations with Statistical Mechanics. **2023**, 16, 2826 ○
- 134 Nanosized Ti-Based Perovskite Oxides as Acid-Base Bifunctional Catalysts for Cyanosilylation of Carbonyl Compounds. **2023**, 15, 17957-17968 ○
- 133 Bayesian optimization with active learning of design constraints using an entropy-based approach. **2023**, 9, ○
- 132 First principles terahertz spectroscopy of molecular crystals: the crucial role of periodic boundary conditions benchmarked with experimental l-ascorbic acid spectra. ○
- 131 Selective synthesis of butane from carbon monoxide using cascade electrolysis and thermocatalysis at ambient conditions. ○
- 130 Molecular insights into the hydration of zwitterionic polymers. ○
- 129 Energy level alignments between organic and inorganic layers in 2D layered perovskites: conjugation vs. substituent. ○
- 128 Adsorption of water and formic acid molecules on the (104) surface of calcite: a theoretical study by DFT-D3. ○
- 127 ??????????????????. ○
- 126 Relative Stability of Pyrazinamide Polymorphs Revisited: A Computational Study of Bending and Brittle Forms Phase Transitions in a Broad Temperature Range. **2023**, 13, 617 ○
- 125 High-Throughput First-Principles Prediction of Interfacial Adhesion Energies in Metal-on-Metal Contacts. **2023**, 15, 19624-19633 ○
- 124 Structural and theoretical investigations on the coloring scheme of brass type phase Ag₅Cd₈. **2023**, 323, 124019 ○
- 123 Molecular orientation-dependent energetic shifts in solution-processed non-fullerene acceptors and their impact on organic photovoltaic performance. **2023**, 14, ○
- 122 Friction properties of black phosphorus: a first-principles study. **2023**, 34, 275703 ○
- 121 A pyrolysis-free Ni/Fe bimetallic electrocatalyst for overall water splitting. **2023**, 14, ○

- 120 General Theory for Bilayer Stacking Ferroelectricity. **2023**, 130, ○
- 119 Heterogeneous Integration of Freestanding Bilayer Oxide Membrane for Multiferroicity. ○
- 118 Revealing the Epitaxial Interface between Al₁₃Fe₄ and Al₅Fe₂ Enabling Atomic Al Interdiffusion. **2023**, 15, 19593-19603 ○
- 117 Methoxy Functionalization of Phenethylammonium Ligand for Efficient Perovskite Light-Emitting Diodes. ○
- 116 Synthesis, Characterization, and Modeling of a Chemically Ordered Quaternary Boride, Mo₄MnSiB₂. ○
- 115 Two-dimensional ferromagnetic semiconductors of rare-earth Janus 2H-GdIBr monolayers with large valley polarization. ○
- 114 Two-dimensional ferroelectricity in a single-element bismuth monolayer. ○
- 113 Density functional theory (DFT) simulation and approach to property-driven investigations in ceramic and composites materials. **2023**, 461-490 ○
- 112 Electrocatalytic reduction of CO₂ on size-selected nanoclusters of first-row transition metal nanoclusters: a comprehensive mechanistic investigation. ○
- 111 Reaction nanoscopy of ion emission from sub-wavelength propanediol droplets. **2023**, ○
- 110 Probing Anisotropic Deformation and Near-Infrared Emission Tuning in Thin-Layered InSe Crystal under High Pressure. ○
- 109 New Zintl Phase Yb₁₀MgSb₉ with High Thermoelectric Performance. ○
- 108 First principles analysis on the nucleation interface of La₂O₃(11 0)/NbC(1. **2023**, 35, 105957 ○
- 107 Robust half-metallicity and topological properties in square-net potassium manganese chalcogenides. **2023**, 107, ○
- 106 Synergistic effect of phosphorus doping and MoS₂ co-catalysts on g-C₃N₄ photocatalysts for enhanced solar water splitting. **2023**, 158, 171-179 ○
- 105 Molecular Understanding of Adhesion of Epoxy Resin to Graphene and Graphene Oxide Surfaces in Terms of Orbital Interactions. **2023**, 39, 5514-5526 ○
- 104 Orbital degree of freedom induced multiple sets of second-order topological states in two-dimensional breathing Kagome crystals. **2023**, 8, ○
- 103 Order-disorder phase transition driven by interlayer sliding in lead iodides. **2023**, 14, ○

- 102 Shock-induced metallization of polystyrene along the principal Hugoniot investigated by advanced thermal density functionals. **2023**, 107,
- 101 Topotactic hydrogen forms chains in ABO₂ nickelate superconductors. **2023**, 107,
- 100 Exploring Proton Pair Motion Away from the Global Proton Triple Energy Minimum in Yttrium-Doped Barium Zirconate. **2023**, 11, 160
- 99 Magnetic Anisotropy of Single-ion Magnet (PPh₄)₂[ReF₆] · 2H₂O.
- 98 Tailoring planar slip to achieve pure metal-like ductility in body-centred-cubic multi-principal element alloys.
- 97 Modulating the Proton-Conducting Lanes in Spinel ZnMn₂O₄ through Off-Stoichiometry.
- 96 Magnetic bond-order potential for iron-cobalt alloys. **2023**, 7,
- 95 Reversible hydrogen storage tendency of light-metal (Li/Na/K) decorated carbon nitride (C₉N₄) monolayer. **2023**,
- 94 Magnetic excitations in infinite-layer LaNiO₂. **2023**, 122, 152401
- 93 Interaction of Bromine with Cu(100) surface: adsorption and thermodynamics stability study.
- 92 Structure and Reactivity of the Ionic Liquid [C₁C₁Im][Tf₂N] on Cu(111).
- 91 First-principles study of electronic and optical properties of novel 2D TiOS monolayer and bilayer: Dimensionality reduction opens up a band gap in TiOS. **2023**, 48, 106438
- 90 The Effect of Hydrogen on Plastic Anisotropy of Mg and β -Ti/Zr from First-Principles Calculations. **2023**, 16, 3016
- 89 Cation disorder dominates the defect chemistry of high-voltage LiMn_{1.5}Ni_{0.5}O₄ (LMNO) spinel cathodes.
- 88 Understanding Li interaction in TiO₂/graphene composites for high-performance Li-ion battery anodes: A first principles study. **2023**, 660, 414878
- 87 Active learning strategies for atomic cluster expansion models. **2023**, 7,
- 86 Mechanism Regulating Self-Intercalation in Layered Materials.
- 85 Morphology-dependent adsorption energetics of Ru nanoparticles on hcp-boron nitride (001) surface: A first-principles study.

- 84 First-principles calculations to investigate optical properties of topological semimetal MX compounds (M = Ti, Zr, Hf and X = S, Se, Te). **2023**, 106001
- 83 Diffusion behavior determined by the new n-body potential in highly immiscible W/Cu system through molecular dynamics simulations. **2023**, 24, 3731-3745
- 82 Pressure-Controlled Layer-by-Layer to Continuous Oxidation of ZrS₂(001) Surface.
- 81 Ab initio calculation of the reflectivity of molecular fluids under shock compression. **2023**, 107,
- 80 Band Gaps and Optical Properties of RENiO₃ upon Strain: Combining First-Principles Calculations and Machine Learning. **2023**, 16, 3070
- 79 Dielectric Saturation in Water from a Long-Range Machine Learning Model.
- 78 Charge transfer driving interfacial reconstructions in perovskite oxide heterostructures. **2023**, 6,
- 77 Formation of intermetallic compounds during reaction between Ti and AlMg alloys with various Mg contents. **2023**,
- 76 Effect of local chemical environment on the point defects in AlNbTiZr refractory high entropy alloys. **2023**, 154451
- 75 Photoemission study of twisted monolayers and bilayers of WSe₂ on graphite substrates. **2023**, 7,
- 74 Band Gap Engineering in Quadruple-Layered Sr_{1-x}Aurivillius Perovskite Oxychlorides Bi₇Fe₂Ti₂O₁₇X (X = Cl, Br, I) for Enhanced Photocatalytic Performance. **2023**, 13, 751
- 73 High quantum oscillation frequencies and nontrivial topology in kagome superconductor KV₃Sb₅ probed by torque magnetometry up to 45 T. **2023**, 107,
- 72 Intrinsic point defects and the n-type dopability of Bi₂MoO₆ with higher photocatalytic performance: A hybrid functional study. **2023**, 7,
- 71 Structural, Elastic, and Mechanical Properties of Orthorhombic Goethite (α-FeOOH) under Pressure from First-Principles Calculations. **2023**, 97, 50-56
- 70 Monte Carlo Simulations of Water Adsorption in Aluminum Oxide Rod-Based Metal-Organic Frameworks.
- 69 Secondary-Phase-Induced Charge-Discharge Performance Enhancement of Co-Free High Entropy Spinel Oxide Electrodes for Li-Ion Batteries.
- 68 Artificial Intelligence Guided Studies of van der Waals Magnets.
- 67 Mechanistic Insights into the High Selectivity and Photocatalytic Activity of Brookite TiO₂ toward NO_x Abatement.

- 66 Insights into Interfacial Structure of Slag/Metal Interface During Desulfurization Through XPS and DFT Simulations. ○
- 65 Effects of Alloying Elements on the Solution and Diffusion of Oxygen at Iron Grain Boundary Investigated by First-Principles Study. **2023**, 13, 789 ○
- 64 Water-assisted sonochemically-induced demethylenation of benzyl alcohol to phenol over a structurally stable cupric oxide catalyst. ○
- 63 Spin-Lattice Coupled Metamagnetism in Frustrated van der Waals Magnet CrOCl. ○
- 62 A molecular understanding of citrate adsorption on calcium oxalate polyhydrates. ○
- 61 Structural transitions at high pressure and metastable phase in Si_{0.8}Ge_{0.2}. **2023**, 170180 ○
- 60 Electrochemical detection of arsenic (III) hazardous chemicals using cubic CsPbBr₃ single crystals: Structural insights from DFT study. **2023**, 115940 ○
- 59 Rise and fall of Mott insulating gaps in YNiO₃ paramagnets as a reflection of symmetry breaking and remaking. **2023**, 7, ○
- 58 Scalable synthesis of coordinatively unsaturated metal-nitrogen sites for large-scale CO₂ electrolysis. **2023**, 14, ○
- 57 Catalytic decomposition of NO using molten gallium: an experimental and computational study. **2023**, 543, 113144 ○
- 56 Green Hydrophobic Deep Eutectic Solvents as Low-Viscosity and Efficient Lubricants. **2023**, 108531 ○
- 55 Elucidating the Effect of Ion Exchange Protocol on the Copper Exchange Efficacy, Copper Siting, and SCR activity in Cu-SSZ-13. ○
- 54 Regulated Surface Electronic States of CuNi Nanoparticles through Metal-Support Interaction for Enhanced Electrocatalytic CO₂ Reduction to Ethanol. ○
- 53 In-Plane Anomalous Hall Effect in PT-Symmetric Antiferromagnetic Materials. **2023**, 130, ○
- 52 Synergetic C-H bond activation and C-D formation on CuOx facilitates facile conversion of methane to methanol. **2023**, 627, 157283 ○
- 51 Role of surface terminations in the chemical stability of CH₃NH₃PbI₃ perovskite in combined light, H₂O, and O₂ environments: DFT/AIMD calculations and experimental validation. **2023**, 18, 100370 ○
- 50 Manipulation of nano-metals to implement rational conduction tailoring for high-efficiency microwave absorption. **2023**, 118045 ○
- 49 Synthesis and Structure of the Double-Layered Sillurivillius Perovskite Oxochloride La_{2.1}Bi_{2.9}Ti₂O₁₁Cl as a Potential Photocatalyst for Stable Visible Light Solar Water Splitting. ○

- 48 Density functional theoretical assessment of titanium metal for adsorption of hydrogen, deuterium and tritium isotopes. **2023**, 142,
- 47 Fe₄ cluster as the smallest 3D Fe cluster with unique quantum magnetic levitation effect on graphene. **2023**, 157315
- 46 Topological Insulator Bi₂Se₃-Assisted Heterostructure for Ultrafast Charging Sodium-Ion Batteries.
- 45 Mechanism of Stoichiometrically Governed Titanium Oxide Brownian Tree Formation on Stepped Au(111).
- 44 Ultralow Lattice Thermal Conductivity and High Thermoelectric Performance in Ge_{1-x}BixCayTe with Ultrafine Ferroelectric Domain Structure.
- 43 A facile method for the preparation of non-metal doped nanotitania featuring visible-region photocatalytic performance. **2023**, 294, 116497
- 42 Breathable MOFs Layer on Atomically Grown 2D SnS₂ for Stable and Selective Surface Activation.
- 41 Protection of Titanium Alloys Against High Temperature Oxidation During Closed-die Forging: Structural Analysis of the Boro-silicate Glass Coating/Ti-6Al-4V Alloy Interfacial Region by Correlative Imaging. **2023**, 111198
- 40 DFT study on termination stabilities of Mg₁₇Al₁₂ (110) surface. **2023**, 33, 755-764
- 39 Large intrinsic anomalous Hall effect in both Nb₂FeB₂ and Ta₂FeB₂ with collinear antiferromagnetism. **2023**, 107,
- 38 High throughput calculations for a dataset of bilayer materials. **2023**, 10,
- 37 Hydrogen and helium trapping in hcp beryllium. **2023**, 6,
- 36 The Mean Inner Potential of Hematite α -Fe₂O₃ Across the Morin Transition.
- 35 Magnetic properties of defect induced β -Ga₂O₃: A first principles study. **2023**, e00810
- 34 Double Perovskite La₂MnNiO₆ as a High-Performance Anode for Lithium-Ion Batteries.
- 33 Construction of the Fast Potassiation Path in Sb_xBi_{1-x}@NC Anode with Ultrahigh Cycling Stability for Potassium-Ion Batteries.
- 32 Thickness-dependent piezoelectricity of black arsenic from few-layer to monolayer. **2023**, 115175
- 31 Irradiation Damage Reduces Alloy Corrosion Rate via Oxide Space Charge Compensation Effects. **2023**, 118956

- 30 Size effect of ruthenium nanoparticles on water cracking properties with different crystal planes for boosting electrocatalytic hydrogen evolution. **2023**, ○
- 29 Consistent wide-range equation of state of silicon by a unified first-principles method. **2023**, 107, ○
- 28 VTaNbAl: A class of spin gapless semiconductors with topological nontrivial features. **2023**, 107, ○
- 27 On the Dopant, Defect States, and Mobility in W Doped Amorphous In₂O₃ for BEOL Transistors. **2023**, ○
- 26 Single-Wall-Carbon-Nanotube/Se₂ Nanohybrid for Ultrafast Visible-To-Near-Infrared Third-Order Nonlinear Optical Limiters. **2023**, 19, ○
- 25 Theoretical Study of Stability of Halogen-Defective Trihalide Monolayers: Cases of AlI₃, AsI₃, and IrBr₃. ○
- 24 Simple Approach for Reconciling Cyclic Voltammetry with Hydrogen Adsorption Energy for Hydrogen Evolution Exchange Current. **2023**, 14, 4164-4171 ○
- 23 Electrochemically stable frustrated Lewis pairs on dual-metal hydroxides for electrocatalytic CO₂ reduction. ○
- 22 Balance between thermal stability and operation speed realized by Ti gradient doping in Sb₂Te₃ phase-change memory. **2023**, 133, ○
- 21 Bismuth Nanoplatelets: Universal Synthetic Strategy and Emerging Application for PEC-Type Photodetectors. **2023**, 100349 ○
- 20 Influencing mechanism of carbon monoxide on the hydrogen absorption performance of Zr₂Fe. **2023**, 466, 143231 ○
- 19 Predicting HP-HT Earth and Planetary Materials. **2023**, 131-151 ○
- 18 Role of hydride ion within Ru/LaScSi and Ru/CeTiGe catalysts for NH₃ synthesis: A combination of DFT and experimental nitrogen isotopic exchange studies. **2023**, 179, 106689 ○
- 17 Atomic-scale investigation on endurance mechanism of the GeTex-based OTS device by Si doping. **2023**, 213, 112127 ○
- 16 A Copper Single-Atom Cascade Bionanocatalyst for Treating Multidrug-Resistant Bacterial Diabetic Ulcer. ○
- 15 Fundamental understanding of C₂H₄ production from C₂H₆ oxidation on stoichiometric IrO₂(1 1 0) surface. **2023**, 631, 157456 ○
- 14 Electrospun CuCoN_{0.6} coating necklace-like N-doped carbon nanofibers for high performance lithium-sulfur batteries. **2023**, 645, 705-714 ○
- 13 Insight into structure, elastic anisotropy, and phonon dispersion relations of Mg₁₇Ce₂ and Mg₄₁Ce₅ alloys. **2023**, 213, 112128 ○

- 12 Impact of Sb degrees of freedom on the charge density wave phase diagram of the kagome metal CsV₃Sb₅. **2023**, 107,
- 11 Pressure-induced antiferromagnetic-tetragonal to nonmagnetic-collapse-tetragonal insulator-metal transition in ThMnAsN.
- 10 Li-ion transport in solid-state electrolyte of Li_{1-x}Al_{1-x}Si_{2+x}O₆: an ab initio study.
- 9 Size-Dependent Structures and Catalytic Properties of Supported Bimetallic PtSn Catalysts for Propane Dehydrogenation Reaction. 7383-7394
- 8 Elastemp DA workflow to compute the quasi-harmonic temperature dependent elastic constants of materials. **2023**, 226, 112223
- 7 Dynamic Formation of Brønsted Acid Sites over Supported WO_x/Pt on SiO₂ Inverse Catalysts-Spectroscopy, Probe Chemistry, and Calculations. 7371-7382
- 6 Predicting properties of high entropy carbides from their respective binaries. **2023**, 226, 112255
- 5 In Silico Demonstration of Fast Anhydrous Proton Conduction on Graphanol.
- 4 Accurate prediction of short-range order and its effect on thermodynamic, structural, and electronic properties of disordered alloys: exemplified in archetypical Cu₃Au. **2023**, 106214
- 3 ANALYSIS OF TiFe INTERMETALLIC COMPOUND BY DFT.
- 2 Three-dimensional porous metal phosphide cathode electrodes prepared via electroless galvanic modification for alkaline water electrolysis.
- 1 Toward using collective x-ray Thomson scattering to study CH demixing and hydrogen metallization in warm dense matter conditions. **2023**, 30,