Crystal orbital Hamilton populations (COHP): energy-resolved visualization of chemical bonding in solids based on density-functional calculations

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2223 Correlating Ion Mobility and Single Crystal Structure in Sodium-Ion Chalcogenide-Based Solid State Fast Ion Conductors: Na11Sn2PnS12 (Pn = Sb, P).

2222 Computational methods in the theory of chemical bonding in solids. **1997**, 38, 459-482 1

2221 A Theoretical Study of Bonding in Lanthanide Trihalides by Density Functional Methods. **1998**, 102, 6812-6820 90

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2219 Metal□Metal Bonding and Metallic Behavior in Some ABO2 Delafossites. **1998**, 10, 2189-2196 57

2218 CePS4 Electronic Structure and Optical Properties. **1998**, 10, 2341-2347 38

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2215	Differences and Similarities between the Isotypic AntimonidesMFe1−xSb, ScCo1−xSb, andMNiSb (M=Zr, Hf). **1999**, 144, 330-338	6
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2213	Der Valenzzustand von Nickel, Zinn und Schwefel im ternären Chalkogenid Ni3Sn2S2 ? XPS-, 61Ni- und 119Sn-Mößbauer-Untersuchungen und Bandstrukturrechnungen. **1999**, 111, 2524-2527	14
2212	Neuartige ternäre Alkalimetallsilberacetylide MIAgC2 (MI=Li, Na, K, Rb, Cs). **1999**, 111, 3697-3700	14
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2210	Novel Ternary Alkali Metal Silver Acetylides MIAgC2 (MI=Li, Na, K, Rb, Cs). **1999**, 38, 3492-3495	27
2209	New binary antimonide Hf5Sb3. **1999**, 291, 73-79	13
2208	InCrBr3: A Ternary Indium Bromide Containing Jahn−Teller Unstable Cr2+ and the Magnetic Structures of InCrBr3 and InFeBr3. **1999**, 38, 2614-2620	1
2207	Where are the Atoms in Quasicrystals? Experimental and Theoretical Studies of Ternary and Quaternary Approximants. **2000**, 643, 311	
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2202	Equiatomic Intermetallic Europium Compounds: Syntheses, Crystal Chemistry, Chemical Bonding, and Physical Properties. **2000**, 12, 875-897	102
2201	Conduction band polarization in some CMR materials: Evolving guidelines for new systems. **2000**, 2, 677-685	18
2200	Developing the MTO Formalism. **1999**, 3-84	12
2199	Ti2Sn3: A Novel Binary Intermetallic Phase, Prepared by Chemical Transport at Intermediate Temperature. **2000**, 12, 2219-2224	23
2198	A Comparative Theoretical Study of the Hydrogen, Methyl, and Ethyl Chemisorption on the Pt(111) Surface. **2000**, 122, 4129-4144	175

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2196	Zr1-xTixSb: A Novel Antimonide on the Quasibinary Section ZrSb□TiSb with a Complex Crystal Structure Exhibiting Linear Sb Chains and Fragments of the TiSb Structure. **2000**, 122, 853-860	39
2195	A unique distortion in K1/3Ba2/3AgTe2: X-ray diffraction determination and electronic band structure analysis of its incommensurately modulated structure. **2000**, 39, 1398-409	9
2194	Electronic structure and magnetism of equiatomic FeN. **2000**, 12, 4161-4173	31
2193	Visualizing the Role of Bi 6s □one Pairs□n the Off-Center Distortion in Ferromagnetic BiMnO3. **2001**, 13, 2892-2899	659
2192	A three-dimensional extended Sb network in the metallic antimonides (M',Ti)5Sb8 (M' = Zr, Hf, Nb, Mo). **2001**, 40, 95-100	25
2191	Ti5Si1.3Sb1.7 ? The first titanium silicide antimonide, forming a crystal structure not found in either binary system. **2001**, 79, 1338-1343	6
2190	Chapter 207 Structure-property relations of ternary equiatomic YbTX intermetallics. **2001**, 32, 453-513	3
2189	Structure Prediction Using Our Semiempirical Structure Map: The Crystal Structure of the New Arsenide ZrTiAs. **2001**, 13, 4053-4057	10
2188	Visualizing lone pairs in compounds containing heavier congeners of the carbon and nitrogen group elements. **2001**, 113, 487-496	32
2187	Electronic Band Structure of TlTe. **2001**, 157, 193-205	5
2186	Extraordinarily Short Pb□Pb Bonds in the New Binary Intermetallic Ti6Pb4.8. **2001**, 159, 134-138	7
2185	Li10Mg6Zn31Al3: A New Intermetallic Phase Containing Building Blocks for Decagonal Quasicrystals. **2001**, 113, 4876-4878	
2184	Ternary alkali metal transition metal acetylides A2MC2 (A = Na, K; M = Pd, Pt). **2001**, 7, 1952-8	27
2183	Li(10)Mg(6)Zn(31)Al(3): A New Intermetallic Phase Containing Building Blocks for Decagonal Quasicrystals The Ames Laboratory is operated for the U.S. Department of Energy (US DOE) by Iowa State University under contract No. W-7405-ENG-82. This work was supported by the Office of Basic Energy Sciences, Materials Chemistry Division of the US DOE. The Bruker CCD-1000	5
2182	Defect clusterization and transport properties of oxide and fluoride ionic conductors with fluorite structure: Quantum-chemical approach. **2001**, 43, 1686-1699	2
2181	Atomic orbital participation on a chemical bond through a binding energy partitioning scheme. **2001**, 549, 9-22	4
2180	Structure and chemical bonding of UAuGe. **2001**, 13, 3123-3137	4

2179	Interpretation ofab initiototal energy results in a chemical language: I. Formalism and implementation into a mixed-basis pseudopotential code. **2001**, 13, 11541-11550	50
2178	Electronic structure, phase stability, and chemical bonding in Th2Al and Th2AlH4. **2002**, 65,	22
2177	Reinvestigation of the Incommensurate Structure of PbO.. **2002**, 755, 1	4
2176	Covalent bonding and bandgap formation in transition-metal aluminides: di-aluminides of group VIII transition metals. **2002**, 14, 5755-5783	41
2175	Chemical bonding variations and electron-phonon interactions. **2002**, 124, 10712-7	14
2174	New layered rubidium rare-earth selenides: syntheses, structures, physical properties, and electronic structures for RbLnSe(2). **2002**, 41, 5716-20	30
2173	The LixVPn4 Ternary Phases (Pn = P, As): Rigid Networks for Lithium Intercalation/Deintercalation. **2002**, 14, 4126-4133	56
2172	Zr(11)Sb(18): a new binary antimonide exhibiting an unusual Sb atom network with nonclassical Sb-Sb bonding. **2002**, 41, 538-45	35
2171	Realistic tight-binding model for the electronic structure of II-VI semiconductors. **2002**, 66,	73
2170	On the electronic structure of the pure and oxygen covered Ru() surface. **2002**, 497, 305-310	4
2169	New quaternary bismuth sulfides: syntheses, structures, and band structures of AMBiS4 (A = Rb, Cs; M = Si, Ge). **2002**, 41, 7094-9	25
2168	The stability range of the CaAl2Si2-type structure in case of LnAl2Ge2 compounds. **2002**, 4, 261-265	28
2167	An ab-initio study of the rˆle of lone pairs in the structure and insulatormetal transition in SnO and PbO. **2002**, 4, 467-474	53
2166	First-principles electronic structure of the delafossites ABO2 (A=Cu, Ag, Au; B=Al, Ga, Sc, In, Y): evolution of d10d10 interactions. **2002**, 4, 1045-1052	50
2165	Chemically tuning between ferromagnetism and antiferromagnetism by combining theory and synthesis in iron/manganese rhodium borides. **2002**, 41, 2528-32	57
2164	Synthesis, Structure, and Thermoelectric Properties of the New Antimonide Sulfide MoSb2S. **2002**, 2002, 591-596	8
2163	Magnetic and Electrical Properties, 151Eu Mssbauer Spectroscopy, and Chemical Bonding of REAgMg (RE=La, Ce, Eu, Yb) and EuAuMg. **2002**, 164, 201-209	39
2162	Intermetallic lithium compounds with two- and three-dimensional polyanionsynthesis, structure, and lithium mobility. **2002**, 13, 506-513	14

2161	Modifying polyacetylene. **2002**, 593, 155-173	6
2160	Crystal structure predictions: the crystal and electronic structure of Zr1−xV1+xAs. **2002**, 169, 96-102	7
2159	Sulfur−Gold Orbital Interactions which Determine the Structure of Alkanethiolate/Au(111) Self-Assembled Monolayer Systems. **2002**, 106, 12727-12736	117
2158	Electronic structure and catalysis on metal surfaces. **2002**, 53, 319-48	801
2157	Preparation, crystal structure and physical properties of ternary compounds (R3N)In, R=rare-earth metal. **2003**, 5, 1247-1257	39
2156	Chemical pressure and hydrogen insertion effects in CeNiIn. **2003**, 5, 1385-1393	16
2155	Ag13OsO6: a silver oxide with interconnected icosahedral Ag134+ clusters and dispersed [OsO6]4- octahedra. **2003**, 42, 4322-5	23
2154	Ba14Zn5−xAl22+x: a new polar intermetallic compound with a novel 2D network. **2003**, 170, 94-105	7
2153	The effect of varying the crystal structure on the magnetism, electronic structure and thermodynamics in the Gd 5 (Si x Ge 1−x) 4 system near x =0.5. **2003**, 171, 57-68	83
2152	Crystallographic, electronic and magnetic studies of Ce4Ni6Al23: a new ternary intermetallic compound in the cerium−nickel−aluminum phase diagram. **2003**, 174, 471-481	15
2151	Sn/Sb atom ordering in the ternary stannide−antimonide TiSnSb. **2003**, 176, 329-337	15
2150	Ground- and excited-state properties of inorganic solids from full-potential density-functional calculations. **2003**, 176, 338-374	9
2149	Syntheses, structures, optical properties, and theoretical calculations of Cs2Bi2ZnS5, Cs2Bi2CdS5, and Cs2Bi2MnS5. **2003**, 174, 334-341	11
2148	The origin of a flat band. **2003**, 176, 412-416	29
2147	Electronic structure, chemical bonding, and spin polarization in ferromagnetic MnAl. **2003**, 176, 390-399	20
2146	Theoretical studies on cerium nickel aluminides: polar intermetallics with heavy fermion behavior. **2003**, 176, 538-548	10
2145	First-principles study of ternary metal borocarbide compounds containing finite linear BC2 units. **2003**, 176, 609-614	17
2144	Density functional study of lanthanide complexes (η5-C5H5)2LnX·OC4H8 (Ln=La−Lu; X=F, Cl, Br and I). **2003**, 679, 84-92	16

2143	N2O interaction with Pd(110): cluster vs. slab model. **2003**, 532-535, 213-220	4
2142	Crystal Chemistry and Electronic Structure of the Metallic Ternary Nitride, SrTiN2. **2003**, 15, 3922-3929	22
2141	Theoretical Study of the Adsorption of Acetylene on the (111) Surfaces of Pd, Pt, Ni, and Rh. **2003**, 107, 217-223	95
2140	Electronic structure and magnetism in half-Heusler compounds. **2003**, 15, 7307-7323	139
2139	Electronic structure, physical properties and ionic mobility of LiAg2Sn. **2003**, 13, 2561-2565	16
2138	Nine hexagonal ca(5)pb(3)z phases in stuffed mn(5)si(3)-type structures with transition metal interstitial atoms z. Problems with classical valence States in possible zintl phases. **2003**, 42, 6673-81	11
2137	First-principles indicators of metallicity and cation off-centricity in the IV-VI rocksalt chalcogenides of divalent Ge, Sn, and Pb. **2003**, 67,	255
2136	A new look at bonding in trialuminides: reinvestigation of TaAl3. **2003**, 42, 8371-6	16
2135	A novel layered niobium oxychloride compound based on Nb2 pairs and Nb6 octahedral clusters: synthesis and crystal and electronic structures of Nb10Cl16O7. **2003**, 42, 8320-7	14
2134	MA(delta)Sb(2-delta) (M = Zr, Hf; A = Si, Ge): a new series of ternary antimonides and not "beta-ZrSb2". **2003**, 42, 7319-25	18
2133	Synthesis, structure, electrical properties, and band structure calculations of TiAsTe. **2003**, 42, 3194-8	6
2132	"Nanoscale zippers" in Gd5(SixGe(1-x))4: symmetry and chemical influences on the nanoscale zipping action. **2003**, 42, 8223-9	33
2131	Synthesis, Structure, and Physical Properties of Mixed Valent Mo2SbS2, the First Superconducting Antimonide-Sulfide. **2003**, 15, 780-786	13
2130	Structure and bonding of Sr3In11: how size and electronic effects determine structural stability of polar intermetallic compounds. **2003**, 42, 7782-8	28
2129	Ab initio investigations in magnetic oxides. **2003**, 31, 239-299	56
2128	Ternary Stannides LiTSn4 (T = Ru, Rh, Ir)Chemical Bonding and Physical Properties. **2003**, 107, 1943-1948	16
2127	Balanced crystal orbital overlap population□ tool for analysing chemical bonds in solids. **2003**, 15, 7751-7761	56
2126	Band-gap tuning by solid-state intercalations of Mg, Ni, and Cu into Mo3Sb7. **2003**, 81, 1157-1163	23

2125	Chemical Bonding and Pseudogap in Zn- and Cd-based Compounds with Complex Hexagonal Structures. **2003**, 805, 146	1
2124	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
2123	Magneto-structural phase transition in Gd5(Si2Ge2) and MnFe(P1/3As2/3) systems. **2003**, 93, 6882-6884	7
2122	Short hydrogen-hydrogen separation in RNiInH1.333(R=La, Ce, Nd). **2003**, 67,	42
2121	Formation Energies of Point Defects in Copper Indium Diselenide Using ab initio Methods. **2003**, 763, 8101	1
2120	Charge and dimensionality effects on the properties of CaNiN. **2004**, 69,	4
2119	Search for metal hydrides with short hydrogen–hydrogen separation: Ab initio calculations. **2004**, 70,	19
2118	Experimental and computational investigation of structure and magnetism in pyrite Co1−xFexS2: Chemical bonding and half-metallicity. **2004**, 70,	57
2117	Ab initio approach of the hydrogen insertion effect on the magnetic properties of YFe2. **2004**, 70,	39
2116	Solvothermal preparation of ferromagnetic sub-micron spinel CuCr2Se4 particles. **2004**, 6, 841-845	18
2115	Crystal and electronic structure of the red semiconductor Ba4LaSbGe3Se13 comprising the complex anion [Ge2Se7Sb2Se4Ge2Se7]14− **2004**, 177, 2249-2254	20
2114	Metallic behavior of the Zintl phase EuGe2: combined structural studies, property measurements, and electronic structure calculations. **2004**, 177, 3545-3552	71
2113	Carbomolybdate(III): Zur Kenntnis von Pr2[Mo2C3] sowie Strukturbeziehungen zu Er2Mo2C3. **2004**, 630, 2277-2286	9
2112	Magnetic properties of Ca-doped SrRuO3 from full-potential calculations. **2004**, 177, 146-158	32
2111	Itinerant ferromagnetism and antiferromagnetism from the perspective of chemical bonding. **2004**, 96, 89-94	20
2110	T-shaped nets of antimony atoms in the binary antimonide Hf5SB9. **2004**, 43, 5260-2	15
2109	T-förmige Netze aus Sb-Atomen in dem binären Antimonid Hf5Sb9. **2004**, 116, 5372-5375	3
2108	The Predicted Structures of the New Pnictides HfMQ in Contrast to ZrMQ (M = Ti, V; Q = P, As). **2004**, 2004, 1183-1189	6

2107	Magnetic and electronic structure of TlCo2S2. **2004**, 177, 2977-2984	13
2106	Insights on the origin of the structural phase transition in BaV10O15 from electronic structure calculations and the effect of Ti-doping on its structure and electrical transport properties. **2004**, 177, 4516-4527	18
2105	Distorted Sb chains in the interlayer region of the antimonide-selenide MoSb2Se. **2004**, 14, 2768	2
2104	LiSr2(NCN)I3: the first empty tetrahedral strontium(II) entity coordinated by carbodiimide units but without strontium-strontium bonding. **2004**, 2302-3	8
2103	Krylov Subspace Method for Molecular Dynamics Simulation Based on Large-Scale Electronic Structure Theory. **2004**, 73, 1519-1524	38
2102	Electronic Structure and Physical Properties of the Semiconducting Polytelluride Ba2SnTe5 with a Unique Te54- Unit. **2004**, 16, 4193-4198	37
2101	Syntheses and structural, physical, and theoretical studies of the novel isostructural Mo9 cluster compounds Ag(2.6)CsMo9Se11, Ag(4.1)ClMo9Se11, and h-Mo9Se11 with tunnel structures. **2004**, 43, 1257-63	20
2100	Planar nets of Ti atoms comprising squares and rhombs in the new binary antimonide Ti2Sb. **2004**, 126, 8295-302	17
2099	Crystal structure and physical properties of a new CuTi2S4 modification in comparison to the thiospinel. **2004**, 43, 6473-8	27
2098	Design of Potential Hydrogen-Storage Materials Using First-Principle Density-Functional Calculations. **2004**, 4, 471-477	50
2097	Band Gap Tuning in New Strontium Seleno-Stannates. **2004**, 16, 2215-2221	29
2096	Crystal structures of Sr4Sn2Se9 and Sr4Sn2Se10 and the oxidation state of tin in an unusual geometry. **2004**, 43, 6830-7	17
2095	Unusual electronic and bonding properties of the Zintl phase Ca5Ge3 and related compounds. A theoretical analysis. **2004**, 126, 5277-81	56
2094	Effect of H insertion on the magnetic, electronic, and structural properties of CeCoSi. **2004**, 70,	49
2093	Covalently bonded 1(infinity)[Pt]- chains in BaPt: extension of the Zintl-Klemm concept to anionic transition metals?. **2004**, 126, 14123-8	47
2092	Electronic structure of defects and defect clusters in narrow band-gap semiconductor PbTe. **2004**, 16, S5277-S5288	19
2091	Metal-metal bonding in ScTaN2. A new compound in the system ScN-TaN. **2004**, 43, 6188-94	19
2090	First-principles electronic structure of spinel LiCr2O4: A possible half-metal. **2004**, 69,	17

2089	Ab initio investigations of TlI-type compounds under high pressure. **2004**, 219,	17
2088	Chemical-bonding and high-pressure studies on hydrogen-storage materials. **2004**, 30, 349-357	27
2087	Crystal structures of R2Pd2Pb (R = Y, La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, and Lu) compounds. **2004**, 370, 217-222	9
2086	A theoretical search for intermetallic compounds and solution phases in the binary system Sn/Zn. **2004**, 379, 110-116	6
2085	Praseodymium diiodide, PrI2, revisited by synthesis, structure determination and theory. **2004**, 380, 211-218	23
2084	Ab initio studies on chemical bonding in Cd- and Zn-based quasicrystals. **2004**, 334-335, 336-341	8
2083	Rare earth□ransition metal□ndides. **2004**, 34, 1-133	40
2082	Synthesis, structure, and electronic structure of K2CuSbS3. **2005**, 178, 3169-3175	24
2081	Ab initio investigation of the magnetic states of Ca2MnO4 and Ca2MnO3.5. **2005**, 310, 231-238	9
2080	Synthesis, crystal and electronic structures of the novel Nd12.4Mg0.6Mo13O36 compound containing Mo13 clusters. **2005**, 8, 1719-1727	2
2079	Structure and Bonding of Li1.42(5)Pd2Sn5.58(5): A Lithium Intercalated Palladium Stannide. **2005**, 17, 911-915	8
2078	Synthesis, structure, and electronic and physical properties of the two SrZrS3 modifications. **2005**, 7, 1049-1054	51
2077	Structure and chemical bonding of Ce2Ge2In and Ce2Pt2In. **2005**, 7, 998-1002	13
2076	Ba(4)Mo(12)S(18): A superconductor containing the dimeric unit (Mo(6))(2)S(24), the missing link between the Mo(6)S(14) and Mo(9)S(17) units. **2005**, 44, 1363-5	7
2075	Dibariumplatinide: (Ba2+)2Pt2-.2e- and its relation to the alkaline-earth-metal subnitrides. **2005**, 44, 770-3	20
2074	Predicting new ferromagnetic nitrides from electronic structure theory: IrFe3N and RhFe3N. **2005**, 44, 1205-10	51
2073	Ba4Mo12S18: A Superconductor Containing the Dimeric Unit (Mo6)2S24, the Missing Link between the Mo6S14 and Mo9S17 Units. **2005**, 117, 1387-1389	1
2072	Dibariumplatinide: (Ba2+)2Pt2□2 e□and Its Relation to the Alkaline-Earth-Metal Subnitrides. **2005**, 117, 780-783	15

2071	Vorhersage neuer ferromagnetischer Nitride auf der Basis von Elektronenstrukturrechnungen: IrFe3N und RhFe3N. **2005**, 117, 1230-1235	9
2070	The new semiconducting polychalcogenide Ba2SnSe5 exhibiting units and distorted SnSe6 octahedra. **2005**, 178, 1087-1093	32
2069	Synthesis, crystal structure, and electronic structure of RbVSe2. **2005**, 178, 3251-3255	1
2068	A High Pressure Study on NH4Pb2Br5 Type Compounds Part II: Electronic Structure and Changes under High Pressure. **2005**, 631, 141-147	2
2067	On the Chemical Bonding in LaPdIn2, LaNiMg2, and LaNiCd2 - Intermetallic Compounds with a Filled Distorted Variant of the CaIn2 Type. **2005**, 631, 451-456	19
2066	B5C5 Anionic Molecules Trapped in a Solid Matrix: The Crystal and Electronic Structures of LaBC. **2005**, 631, 1041-1046	18
2065	First-Principles Electronic Structure, Chemical Bonding, and High-Pressure Phase Prediction of the Oxynitrides of Vanadium, Niobium, and Tantalum. **2005**, 631, 887-893	32
2064	(A19N7)[In4]2 (A = Ca, Sr) and (Ca4N)[In2]: Synthesis, Crystal Structures, Physical Properties, and Chemical Bonding. **2005**, 631, 1477-1486	10
2063	The First Titanium Molybdenum Antimonide: Ti5.42Mo2.58Sb9, a Substitution Variant of Zr2V6Sb9. **2005**, 631, 1924-1928	3
2062	Interlayer contraction in MgB2 upon replacement of Mg by Al: Effect of the covalent bond energy. **2005**, 72,	12
2061	Interatomic bonding, elastic properties, and ideal strength of transition metal aluminides: A case study for Al3(V,Ti). **2005**, 71,	61
2060	Structural stability, electronic structure, and magnetic properties of mixed-valence ACr3O8 phases (A=Na, K, Rb). **2005**, 72,	4
2059	Electronic structure of the antiferromagnetic semiconductor MnSb2S4. **2005**, 71,	18
2058	Nonmetal ordering in TiC1□Nx: Ground-state structure and the effects of finite temperature. **2005**, 72,	15
2057	Theory of large-scale electronic structure calculation and nanoscale mechanical property in fracture behavior of silicon. **2005**, 880, 1	
2056	Ab initio investigation of the nitrofluoride SiNF. **2005**, 72,	6
2055	New Quaternary Barium Copper/Silver Selenostannates: Different Coordination Spheres, Metal□Metal Interactions, and Physical Properties. **2005**, 17, 2255-2261	84
2054	Electron-precise/deficient La(5-x)Ca(x)Ge4 (3.4 2005, 127, 15682-3	43

2053	A New Superstructure for the BaAl4-Structure Type: An Experimental and Theoretical Study of La2NiAl7. **2005**, 17, 3661-3667	23
2052	Importance of cations in the properties of Zintl phases: the electronic structure of and bonding in metallic Na6TlSb41. **2005**, 44, 5636-40	15
2051	Unique Barium Selenostannate Selenide: Ba7Sn3Se13 (and Its Variants Ba7Sn3Se13-xTex) with SnSe4 Tetrahedra and Isolated Se Anions. **2005**, 17, 4509-4513	19
2050	Crystal structures, electronic properties, and pressure-induced superconductivity of the tetrahedral cluster compounds GaNb(4)S(8), GaNb(4)Se(8), and GaTa(4)Se(8). **2005**, 127, 8732-40	74
2049	The indium subnitrides Ae6In4(InxLiy)N(3-z)(Ae = Sr and Ba). **2005**, 44, 6680-90	10
2048	The magnetic structure of TlCrTe2. **2005**, 403, 71-75	7
2047	The coloring problem in intermetallics: bonding and properties of Tb3Zn3.6Al7.4 with the La3Al11 structure type. **2005**, 220,	9
2046	Wurtzite CoO. **2005**, 17, 834-838	90
2045	Preparation, phase stability and structure of the C36 Laves phase Nb1-xCo2+x. **2006**, 221,	17
2044	Ti2Rh6B a new boride with a double perovskite-like structure containing octahedral Rh6 clusters. **2006**, 221,	20
2043	First-principles electronic structure study of the monoclinic crystal bismuth triborate BiB3O6. **2006**, 110, 19254-63	35
2042	New synthesis route to and physical properties of lanthanum monoiodide. **2006**, 45, 2068-74	14
2041	A model study for the breaking of cyanogen out of CNx within DFT. **2006**, 15, 1609-1613	8
2040	Synthesis of a missing structural link: the first trigonal planar B4 units in the novel complex boride Ti(1+x)Os(2-x)RuB2 (x = 0.6). **2006**, 4419-21	31
2039	Structural stability and pressure-induced phase transitions in MgH2. **2006**, 73,	134
2038	Covalent bonding and the nature of band gaps in some half-Heusler compounds. **2006**, 39, 776-785	215
2037	(La3Zx)Al and (Ce3Zx)Al with Z = C, N, O: preparation, physical properties and chemical bonding of metal-rich perovskites. **2006**, 221,	14
2036	Synthesis and crystal and electronic structures of the Na2(Sc4Nb2)(Nb6O12)3 octahedral niobium cluster oxide. Structural correlations between AnBM6L12(Z) series and Chevrel Phases. **2006**, 45, 883-93	10

2035	Intergrowth Compounds in the Zn-Rich ZnPd System: Toward 1D Quasicrystal Approximants. **2006**, 18, 1848-1856	32
2034	Electronic structures of KNa3In9 and Na2In, two metallic phases with classical closed-shell electronic configurations. **2006**, 45, 2960-4	4
2033	La2TeI2: a new layered telluride iodide with unusual electrical properties. **2006**, 45, 10728-33	9
2032	Thermoelectric Properties of the New Polytelluride Ba3Cu14-Te12. **2006**, 18, 3866-3872	37
2031	Unusual Mn-Mn spin coupling in the polar intermetallic compounds CaMn2Sb2 and SrMn2Sb2. **2006**, 45, 4047-54	55
2030	Localized and delocalized chemical bonding in the compounds CaNiGe2, SrNiGe2, and SrNiSn2. **2006**, 45, 7408-16	24
2029	Ba11Cd8Bi14: bismuth zigzag chains in a ternary alkaline-earth transition-metal Zintl phase. **2006**, 45, 7126-32	26
2028	Electronic structure of half-metallic magnets. **2006**, 36, 96-101	12
2027	Crystal structure, electronic structure and thermoelectric properties of Cu4Sn7S16. **2006**, 417, 55-59	27
2026	Crystal and electronic structures and physical properties of two semiconductors: Pb4Sb6Se13 and Pb6Sb6Se17. **2006**, 14, 198-207	14
2025	Intermetallic compounds with 1D infinite tunnels. Syntheses and structures of AAu4In2 (A = K, Rb). **2006**, 128, 12392-3	37
2024	119Sn Mssbauer Spectroscopy and Chemical Bonding in AuTSn2 (T = Ni, Cu, Pd). **2006**, 632, 1432-1436	8
2023	Modeling of hydrogen storage materials by density-functional calculations. **2006**, 159, 88-99	30
2022	Two new titanium molybdenum arsenides: Ti2MoAs2 and Ti3MoAs3, ternary substitution variants of V3As2 and V4As3. **2006**, 179, 464-469	3
2021	Structural, magnetic, and spectroscopic studies of YAgSn, TmAgSn, and LuAgSn. **2006**, 179, 2376-2385	32
2020	Crystal structure, electronic structure and physical properties of the new low-valent thallium silicon telluride Tl6Si2Te6 in comparison to Tl6Ge2Te6. **2006**, 179, 2707-2713	9
2019	Temperature-dependent crystallographic studies and electronic structure of Ba2Cd3Bi4. **2006**, 179, 3371-3377	10
2018	Changes of the magnetic interactions in TlCo2Se2 upon metal substitution. **2006**, 303, 204-213	4

2017	Portraits of some representatives of metal boride carbide and boride silicide compounds. **2006**, 179, 2779-2786	19
2016	CuAl2 revisited: Composition, crystal structure, chemical bonding, compressibility and Raman spectroscopy. **2006**, 179, 1707-1719	84
2015	Structure property relationships in the ATi2O4 (A=Na, Ca) family of reduced titanates. **2006**, 179, 3489-3499	11
2014	Lone pairs in insulating pyrochlores: Ice rules and high-k behavior. **2006**, 8, 259-266	57
2013	A new low temperature modification of TaTe2□comparison to the room temperature and the hypothetical 1T-TaTe2 modification. **2006**, 41, 987-1000	22
2012	Mo(15)S(20): first evidence of a new molybdenum cluster type in a metastable solid-state compound. **2006**, 12, 8513-7	1
2011	Unusual lone pairs in tellurium and their relevance for superconductivity. **2006**, 45, 599-602	15
2010	Mysterious platinum nitride. **2006**, 45, 4365-8	52
2009	Transition-metal anions in solids and their implications on bonding. **2006**, 45, 7465-9	37
2008	Crystal Structure and Properties of MgCo4Ge6. **2006**, 2006, 3482-3488	10
2007	Electronic structure, chemical bonding, and finite-temperature magnetic properties of full Heusler alloys. **2006**, 27, 90-102	21
2006	Ungew□nliche freie Elektronenpaare in Tellur und ihre Bedeutung f□.die Supraleitf□higkeit. **2006**, 118, 613-617	2
2005	Geheimnisvolles Platinnitrid. **2006**, 118, 4472-4476	15
2004	□bergangsmetallanionen in Festk□pern und ihre chemische Bindung. **2006**, 118, 7627-7630	9
2003	Non-icosahedral ordering of transition elements in Zn□M□c quasicrystals. **2006**, 86, 693-699	3
2002	Geometric variations and electron localizations in intermetallics: PbFCl type compounds. **2006**, 221,	23
2001	Electronic structure and magnetic properties of cubic and hexagonal SrMnO3. **2006**, 74,	130
2000	Linear algebraic calculation of the Green□ function for large-scale electronic structure theory. **2006**, 73,	42

1999	Electronic Structure of Solids. **2006**,	1
1998	Electronic and magnetic properties and chemical bonding of CeMSn (M=Rh,Ru) from first principles. **2007**, 76,	38
1997	First-principles study of the electronic and magnetic structures of the tetragonal and orthorhombic phases of Ca3Mn2O7. **2007**, 76,	20
1996	Electronic structure, chemical bonding, and magnetic properties in the intermetallic series Sc2Fe(Ru1□Rhx)5B2 from first principles. **2007**, 76,	39
1995	Two-stage formation model and helicity of gold nanowires. **2007**, 99, 125507	28
1994	Ab initio studies of magnetic properties of cobalt and tetracobalt nitride Co4N. **2007**, 75,	60
1993	Ab initio analysis of magnetovolume versus chemical effects in CeRuSi and its hydride. **2007**, 75,	15
1992	Systematic study on the pressure dependence of M2AlC phases (M=Ti,V,Cr,Zr,Nb,Mo,Hf,Ta,W). **2007**, 76,	62
1991	Ab initio study of ductility in M2AlC (M=Ti, V, Cr). **2007**, 75,	105
1990	Structure, ordering, and bonding of half antiperovskites: PbNi3/2S and BiPd3/2S. **2007**, 35, 309-327	41
1989	On the existence of Ca2Bi-crystal and electronic structure of Ca4Bi2O. **2007**, 427, 67-72	12
1988	Ab initio studies of the electronic structure of the quaternary system LiBC4N4. **2007**, 427, 61-66	4
1987	Electronic structure and chemical bonding in half-Heusler phases. **2007**, 439, 37-54	67
1986	Thermoelectric properties of the new tellurides SrSc2Te4 and BaSc2Te4 in comparison to BaY2Te4. **2007**, 15, 371-376	7
1985	Structure and bonding in SnWO4, PbWO4, and BiVO4: lone pairs vs inert pairs. **2007**, 46, 3839-50	252
1984	Electronic Effects in CO Chemisorption on Pt□b Intermetallic Surfaces: A Theoretical Study. **2007**, 111, 17357-17369	17
1983	Atomic distributions in the gamma-brass structure of the Cu-Zn system: a structural and theoretical study. **2007**, 46, 251-60	63
1982	Structures and physical properties of new semiconducting polyselenides Ba2CudeltaAg4-deltaSe5 with unprecedented linear Se(3)4- units. **2007**, 46, 9906-11	34

1981	Structures and physical properties of new semiconducting gold and copper polytellurides: Ba7Au2Te14 and Ba6.76Cu2.42Te14. **2007**, 46, 1215-21	21
1980	Synthesis, Structure, and Electronic and Physical Properties of Tl2TeS3, the First Characterized Thallium(I) Thiotellurate(IV). **2007**, 19, 221-228	10
1979	Phase transition in Tl2TeO3: influence and origin of the thallium lone pair distortion. **2007**, 46, 446-52	13
1978	Crystal Structure, Electronic Structure, and Physical Properties of Two New Antimonide Tellurides: ZrSbTe and HfSbTe. **2007**, 19, 1482-1488	17
1977	On the origin of a band gap in compounds of diamond-like structures. **2007**, 46, 1957-9	24
1976	Thallium Halides New Aspects of the Stereochemical Activity of Electron Lone Pairs of Heavier Main-Group Elements. **2007**, 2007, 882-890	35
1975	Nd2[MoC2] and RE2[WC2], RE = Ce, Pr, Nd: New carbometalates with Pr2[MoC2] structure type. **2007**, 8, 364-370	1
1974	Local structure and influence of bonding on the phase-change behavior of the chalcogenide compounds K1 RbxSb5S8. **2007**, 180, 420-431	18
1973	Chemical bonding in EuTGe (T=Ni, Pd, Pt) and physical properties of EuPdGe. **2007**, 180, 533-540	10
1972	Ternary rare earth and actinoid transition metal carbides viewed as carbometalates. **2007**, 180, 636-653	41
1971	Condensed rare-earth metal-rich tellurides. Extension of layered Sc6PdTe2-type compounds to yttrium and lutetium analogues and to Y7Te2, the limiting binary member. **2007**, 180, 3172-3179	12
1970	Die Seltenerdmetallpolyselenide Gd8Se15, Tb8Se15 , Dy8Se15 , Ho8Se15 , Er8Se15 und Y8Se15 (0 2007, 633, 261-273	16
1969	Crystal and Electronic Structures of the New Carbomolybdates(III), RE2[Mo2C3] with RE = Ce, Sm, Tb, and Dy. **2007**, 633, 1349-1358	2
1968	Substitution Effects in Zintl Phases: Synthesis and Crystal Structure of the Novel Phases Ae3Sn4 Bi1+x (x 1; Ae = Sr, Ba) Containing Shubnikov-Type Nets $^{2}_{infty}rm [Sn_{4-x}Bi_{x}]$. **2007**, 633, 1568-1574	4
1967	Inkommensurabel modulierte Kristallstrukturen und Phasenumwandlungen Die Verbindungen SrPt2As2 und EuPt2As2. **2007**, 633, 2037-2045	37
1966	Preparation and characterization of Pd2Sn nanoparticles. **2007**, 42, 1969-1975	13
1965	Ab initio investigation of the electronic structures of ternary germanides CeRhGe and CeIrGe. **2007**, 9, 274-278	21
1964	Crystal chemistry and electronic structure of the metallic lithium ion conductor, LiNiN. **2007**, 129, 1912-20	19

1963	Planar versus puckered nets in the polar intermetallic series EuGaTt (Tt = Si, Ge, Sn). **2007**, 46, 8801-11	30
1962	Synthesis, structure and electronic structure of a new polymorph of CaGe2. **2007**, 180, 1575-1581	48
1961	Phase stabilities of monoclinic oxoborates LaB3O6 and GdB3O6 in C121 and I12/a1 phase□Energetics and chemical bonds derived from first-principles calculations. **2007**, 180, 2763-2774	2
1960	Chemical bonding analysis and properties of La7Os4C9□A new structure type containing C- and C2-units as Os-coordinating ligands. **2008**, 181, 3121-3130	22
1959	Syntheses and Structures of the Germanides CaNiGe and MgCoGe as well as Chemical Bonding in CaNiGe and CaNi2Ge2. **2008**, 634, 1249-1255	27
1958	Magnetic, Optical, and Electronic Properties of the Phosphide Oxides REZnPO (RE = Y, La□Nd, Sm, Gd, Dy, Ho). **2008**, 634, 1339-1348	32
1957	SrNi2Ge and SrNi3Ge2 □Two Related Hexagonal Germanides. **2008**, 634, 2316-2322	14
1956	Electronic Structure and Physical Properties of Hf5Sb9 containing a Unique T Net of Sb Atoms. **2008**, 634, 2367-2372	5
1955	Polar intermetallic compounds as catalysts for hydrogenation reactions: synthesis, structures, bonding, and catalytic properties of Ca(1-x)Sr(x)Ni4Sn2 (x=0.0, 0.5, 1.0) and catalytic properties of Ni3Sn and Ni3Sn2. **2008**, 14, 3737-44	20
1954	First-principles and molecular-dynamics study of structure and bonding in perovskite-type oxynitrides ABO(2)N (A = Ca, Sr, Ba; B = Ta, Nb). **2008**, 29, 2260-7	55
1953	Unusual Sb-Sb bonding in high temperature thermoelectric materials. **2008**, 29, 2134-43	38
1952	Analysis of electronic structures and chemical bonding of metal-rich compounds. I. Density functional study of Pt metal, LiPt2, LiPt, and Li2Pt. **2008**, 29, 2154-60	10
1951	Relation between chemical bonding and exchange coupling approaches to the description of ordering in itinerant magnets. **2008**, 29, 2177-86	11
1950	Calcium d States: chemical bonding of CaC6. **2008**, 47, 6703-6	17
1949	Calcium d States: Chemical Bonding of CaC6. **2008**, 120, 6805-6808	8
1948	Structure and physical properties of the new telluride BaAg2Te2 and its quaternary variants BaCu□Ag2□Te2. **2008**, 181, 2024-2030	28
1947	Effect of Cr on the electronic structure of Co3Al intermetallic compound: A first-principles study. **2008**, 320, 1345-1351	13
1946	Ductility improvement of amorphous steels: Roles of shear modulus and electronic structure. **2008**, 56, 88-94	169

1945	Ab initio investigation of perovskite and post-perovskite CaPtO3. **2008**, 352, 92-96	6
1944	On the "coloring problem" in YMgZn and related phases. **2008**, 361, 3053-3062	13
1943	Interplay of negative pressure and hydrogen chemical effects in CeRhSn from first principles. **2008**, 65, 491-498	5
1942	Centrosymmetric silicide ScNiSi3 : structure, chemical bonding, and 45Sc solid state NMR. **2008**, 10, 544-549	6
1941	Crystal and electronic structure of La3Zn2.5P4 : New phosphide with isolated P3 species. **2008**, 10, 1006-1011	13
1940	Structure and properties of RERhZn (RE = La, Ce, Pr, Nd). **2008**, 10, 1895-1904	18
1939	Structural, thermal, and electrical properties of CrSi2. **2008**, 103, 113516	66
1938	An application of the "coloring problem": structure-composition-bonding relationships in the magnetocaloric materials LaFe13-xSix. **2008**, 47, 515-28	49
1937	Searching for hexagonal analogues of the half-metallic half-HeuslerXYZcompounds. **2008**, 41, 035002	24
1936	Thermoelectric properties of Nb3Sb2Te5. **2008**, 448, 148-152	8
1935	Prediction of composition for stable half-Heusler phases from electronic-band-structure analyses. **2008**, 458, 47-60	30
1934	Hydrogen insertion effects on the magnetic properties and chemical bonding within C14 Laves phases. **2008**, 36, 192-212	6
1933	The SIESTA method; developments and applicability. **2008**, 20, 064208	364
1932	Nitridogermanate nitrides Sr7[GeN4]N2 and Ca7[GeN4]N2: synthesis employing sodium melts, crystal structure, and density-functional theory calculations. **2008**, 47, 12018-23	10
1931	Synthesis, structure, and bonding of Sc4MgxCu15-xGa approximately 7.5 (x=0, 0.5). Two incommensurately modulated scandium substitution derivatives of cubic Mg2Cu6Ga5. **2008**, 47, 1020-9	8
1930	An experimental and theoretical study of the variation of 4f hybridization across the La1-xCexIn3 series. **2008**, 47, 2569-75	1
1929	Orbital interpretation of kinetic energy density and a direct space comparison of chemical bonding in tetrahedral network solids. **2008**, 112, 7705-16	4
1928	Crystal Structure, Chemical Bonding, and Magnetic Hyperfine Interactions in GdRu2SiC. **2008**, 20, 1381-1389	3

1927	Ladders of a magnetically active element in the structure of the novel complex boride Ti9Fe2Ru18B8: synthesis, structure, bonding, and magnetism. **2008**, 47, 2113-20	39
1926	Can undoped calcium tetraborides exist? An answer from the comparison of its density functional theory electronic structure with that of rare-earth metal tetraboride. **2008**, 47, 6137-43	11
1925	Cation substitution effects in the system Sr2-xBaxBi3 (0 2008, 47, 3594-602	7
1924	Two-dimensional superdegeneracy and structure-magnetism correlations in strong ferromagnet, Mn2Ga5. **2008**, 130, 1384-91	14
1923	Synthesis, structure, and bonding of the Zintl phase Ba3Cd2Sb4. **2008**, 47, 11237-44	43
1922	Electronic Structure Study of the [Ag4]4-, [Au4]4-, and [Hg]2 2- Zintl Anions in the Intermetallic Compounds Yb3Ag2, Ca5Au4, and Ca3Hg2: Transition Metal Anions As p-Metal Elements. **2008**, 20, 2751-2756	28
1921	First-principles studies for structural transitions in ordered phase of cubic approximant Cd6Ca. **2008**, 20, 315206	12
1920	First principles study of the electronic and magnetic structures of U2Ni2SnH2. **2008**, 10, 083013	4
1919	Crystal structure prediction of LiBeH3 using ab initio total-energy calculations and evolutionary simulations. **2008**, 129, 234105	16
1918	Mechanical properties, glass transition temperature, and bond enthalpy trends of high metalloid Fe-based bulk metallic glasses. **2008**, 92, 161910	44
1917	Chapter 6 Electronic structures and stability mechanism of quasicrystals. **2008**, 171-208	8
1916	Development of the simulation package 'ELSES' for extra-large-scale electronic structure calculation. **2009**, 21, 064233	5
1915	Chemical bonding and mechanical properties of M2AC (M = Ti, V, Cr, A = Al, Si, P, S) ceramics from first-principles investigations. **2009**, 24, 556-564	21
1914	Investigation of changes in crystal and electronic structures by hydrogen within LaNi5 from first-principles. **2009**, 11, 1098-1106	15
1913	Structure, chemical bonding, and 45Sc solid state NMR of Sc2RuSi2. **2009**, 11, 1239-1245	6
1912	Electronic structure and chemical bonding properties of UO2F2 from first principles. **2009**, 11, 1380-1385	4
1911	Synthesis and characterization of quaternary selenides Sn2Pb5Bi4Se13 and Sn8.65Pb0.35Bi4Se15. **2009**, 11, 1666-1672	7
1910	X-ray/neutron diffraction studies and ab initio electronic structure of CeMgNi4 and its hydride. **2009**, 11, 1971-1978	29

1909	Chemistry and Physical Properties of the Phosphide Telluride Zr2PTe2. **2009**, 2009, 3102-3110	17
1908	A combinatorial study of inverse Heusler alloys by first-principles computational methods. **2010**, 31, 612-9	69
1907	Structural and compositional investigations of Zr4Pt2O: A filled-cubic Ti2Ni-type phase. **2009**, 182, 1708-1712	2
1906	Cations Insertion in Molybdenum Cluster Compounds: Electronic Structure and Electrochemical Study Using Cavity Microelectrode. **2009**, 20, 133-143	1
1905	Synthesis and Crystal Structures of NiPdTe and Ni2PdSe2. **2009**, 635, 48-52	2
1904	New Germanium-rich Compounds SrCo5−xGe9 (x = 0.39 and 0.28) with Optimized Co−Ge Bonding. **2009**, 635, 708-716	5
1903	Influence of Element Substitution on the Cluster Arrangement in the Novel Structures Ca3Tl5, Sr3Tl5, and Sr3Sn5−xTlx (x = 1.8 and 2.2)´. **2009**, 635, 1925-1932	6
1902	Synthesis, Crystal and Electronic Structure of a Samarium Carbochromate(III), Sm2[Cr2C3]´. **2009**, 635, 1741-1745	2
1901	Crystal, electronic structures and photoluminescence properties of rare-earth doped LiSi2N3. **2009**, 182, 301-311	56
1900	Synthesis and characterization of quaternary chalcogenides InSn2Bi3Se8 and In0.2Sn6Bi1.8Se9. **2009**, 182, 1450-1456	23
1899	Structure−composition sensitivity in Metallic Zintl phases: A study of Eu(Ga1−xTtx)2 (Tt=Si, Ge, 0≤x≤1). **2009**, 182, 2430-2442	13
1898	Slater−Pauling behavior within quaternary intermetallic borides of the Ti3Co5B2 structure-type. **2009**, 182, 2613-2619	3
1897	Electronic band structure of from first principles. **2009**, 182, 2678-2684	9
1896	BaHg2Tl2. An unusual polar intermetallic phase with strong differentiation between the neighboring elements mercury and thallium. **2009**, 131, 8677-82	14
1895	Synthesis, structure, and bonding in K12Au21Sn4. A polar intermetallic compound with dense Au20 and open AuSn4 layers. **2009**, 48, 11108-13	13
1894	Gold tetrahedra as building blocks in K3Au5Tr (Tr = In, Tl) and Rb2Au3Tl and in other compounds: a broad group of electron-poor intermetallic phases. **2009**, 48, 6573-83	43
1893	Synthesis and phase width of quaternary selenides Pb4In(x)M(6-x)Se13 (M = Bi, x = 2.1-2.8; Sb, x = 2). **2009**, 48, 6402-8	8
1892	Crystal Structure and Physical Properties of the New Selenide−Tellurides Ba3Cu17−x(Se,Te)11. **2009**, 21, 88-93	15

1891	Synthesis, electronic and crystal structures, and physical studies of the superconductor Cs(~1)Mo12S14, final step of the condensation of the Mo6L8(i)L6(a) unit. **2009**, 48, 8337-41	6
1890	Theoretical interpretation of the structural variations along the Eu(Zn(1-x)Ge(x))2 (0 2009, 48, 6391-401	12
1889	Na6ZnSn2, Na4.24K1.76(1)ZnSn2, and Na20Zn8Sn11: three intermetallic structures containing the linear {Sn-Zn-Sn}6- unit. **2009**, 131, 1469-78	25
1888	Electronic structure of the A(8)Tr(11) (A = K, Rb, Cs; Tr = Ga, In, Tl) Zintl phases: possible chemical reasons behind their activated versus non activated conductivity. **2009**, 48, 9792-9	4
1887	Syntheses, crystal and electronic structures, and physical properties of two quaternary chalcogenides: La(4)FeSb(2)Q(10) (Q = S, Se). **2009**, 48, 11518-24	45
1886	Synthesis and characterization of Na5M(2+x)Sn(10-x) (x approximately = 0.5, M = Zn, Hg)--a doped tetrahedral framework structure. **2009**, 131, 10246-52	13
1885	EuAgxAl11□ with the BaCd11-Type Structure: Phase Width, Coloring, and Electronic Structure. **2009**, 21, 230-236	11
1884	Oxide nitrides: From oxides to solids with mobile nitrogen ions. **2009**, 37, 81-131	58
1883	Theory and computer simulation of perfect and defective solids. **2009**, 37, 70-80	4
1882	Density Functional Theory Calculations for Phase Change Materials. **2009**, 17-38	
1881	Noncentrosymmetric Polar Oxide Material, Pb3SeO5: Synthesis, Characterization, Electronic Structure Calculations, and Structure□Property Relationships. **2009**, 21, 5335-5342	124
1880	Theoretical Study of the Role of Indium on the Selectivity of Acrolein Hydrogenation to Propenol on Gold Surfaces. **2009**, 113, 12325-12330	12
1879	Effects of bond character on the electronic structure of brownmillerite-phase oxides, Ca2B?xFe2□O5 (B? = Al, Ga): an X-ray absorption and electron energy loss spectroscopic study. **2009**, 19, 9213	22
1878	A computational study on molecular adsorption states of nitrogen on a tungsten tetramer. **2009**, 11, 943-9	3
1877	New Polar Oxides: Synthesis, Characterization, Calculations, and Structure□Property Relationships in RbSe2V3O12 and TlSe2V3O12. **2009**, 21, 1654-1662	107
1876	R(5)Pn(3)-type phases of the heavier trivalent rare-earth-metal pnictides (Pn = Sb, Bi): new phase transitions for Er(5)Sb(3) and Tm(5)Sb(3). **2009**, 48, 4362-71	10
1875	Comparative Study of Charged and Neutral Oxygen Vacancies in Cubic Zirconia from First Principles. **2009**, 2, 061402	10
1874	Competing structural ordering tendencies in Heusler-type alloys with high Curie temperatures: Fe2CoGa1□Znx studied by first-principles calculations. **2010**, 82,	24

1873	Intermetallic hydrides: A review with ab initio aspects. **2010**, 38, 1-37	71
1872	YNi and its hydrides: Phase stabilities, electronic structures and chemical bonding properties from first principles. **2010**, 377, 109-114	4
1871	Experimental and theoretical studies of Sn3□Pb□Bi2Se6 (□=0.0□0.7). **2010**, 183, 807-813	7
1870	Zr2Ir6B with an eightfold superstructure of the cubic perovskite-like boride ZrIr3B0.5: Synthesis, crystal structure and bonding analysis. **2010**, 183, 784-788	19
1869	Synthesis and structural characterization of A3In2Ge4 and A5In3Ge6 (A=Ca, Sr, Eu, Yb)□New intermetallic compounds with complex structures, exhibiting Ge□Ge and In□In bonding. **2010**, 183, 1258-1265	14
1868	3D [Ag□Mg] polyanionic frameworks in the La4Ag10Mg3 and La4Ag10.3Mg12 new ternary compounds. **2010**, 183, 2995-3001	11
1867	Study of Vacancies and Pd Atom Decoration on the Electronic Properties of Bilayer Graphene. **2010**, 23, 1543-1550	5
1866	Crystal structure, electronic structure and electrical conductivity of the antimony selenide BaLaSb2Se6. **2010**, 12, 919-923	7
1865	AMoO4 (A´=´Mg, Ni) molybdates: Phase stabilities, electronic structures and chemical bonding properties from first principles. **2010**, 12, 1779-1785	31
1864	Studies regarding the homogeneity range of the zirconium phosphide telluride Zr2+□PTe2. **2010**, 12, 2030-2035	5
1863	A density-functional study of the phase diagram of cementite-type (Fe,Mn)3C at absolute zero temperature. **2010**, 31, 2620-7	8
1862	A Bismuth-Stabilized Metal-Rich Telluride Lu9Bi□.0Te□.0 □Synthesis and Characterization. **2010**, 2010, 2620-2625	1
1861	Eight-Coordinate Endohedral Rhenium, Osmium and Iridium Atoms in Rare-Earth Halide Cluster Complexes. **2010**, 2010, 2613-2619	13
1860	On a TiNiSi-Type Superstructure: Synthesis, Crystal and Electronic Structures of CaAgGe and Its Mn-Substituted Derivative. **2010**, 2010, 4139-4147	8
1859	Planar Fe6 Cluster Units in the Crystal Structure of RE15Fe8C25 (RE=Y, Dy, Ho, Er). **2010**, 122, 5824-5828	11
1858	Planar Fe6 cluster units in the crystal structure of RE15Fe8C25 (RE=Y, Dy, Ho, Er). **2010**, 49, 5688-92	16
1857	Dependence of the lone pair of bismuth on coordination environment and pressure: An ab initio study on Cu4Bi5S10 and Bi2S3. **2010**, 183, 2133-2143	35
1856	Synthesis and phase width of new quaternary selenides PbxSn6□Bi2Se9 (x=0□.36). **2010**, 183, 2616-2622	5

1855	Structure, bonding, and magnetic response in two complex borides: Zr2Fe1□Ru5+□B2 and Zr2Fe1□(Ru1□Rhx)5+□B2. **2010**, 183, 2917-2924	20
1854	cis-trans Germanium chains in the intermetallic compounds ALi1□InxGe2 and A2(Li1□Inx)2Ge3 (A=Sr, Ba, Eu)□xperimental and theoreticalstudies. **2010**, 183, 2895-2902	18
1853	New quaternary Zintl phases □Synthesis, crystal and electronic structures of KA2Cd2Sb3 (A = Ca, Sr, Ba, Eu, Yb). **2010**, 29, 456-462	21
1852	Zigzag Chains of Alternating Atoms in A2AuBi (A = Na, K) and K2AuSb. Synthesis, Structure, and Bonding´. **2010**, 636, 67-73	13
1851	Crystal Structure and Physical Properties of RbNb4Br11´. **2010**, 636, 50-53	2
1850	Modulated Lanthanum Chains in the Crystal Structure of La3.65[Ru(C2)3]´. **2010**, 636, 41-49	4
1849	Synthesis, Structure, and Bonding of Ca2Ni3Ge2 and Comparison with CaNiGe, SrNi2Ge, and Ca3Ni3Si2´. **2010**, 636, 100-107	8
1848	Ternary Silicides Sc3TSi3 (T = Ru, Rh, Ir, Pt) □Structure, Chemical Bonding, and Solid State NMR´. **2010**, 636, 1839-1850	10
1847	Synthesis, Structure and Chemical Bonding of CaCo2Si2 and BaCo2Ge2 □Two New Compounds with ThCr2Si2 Structure Type´. **2010**, 636, 378-384	13
1846	The metastable m-Ba2SnSe5 □Synthesis, Phase Transition, Crystal Structure, Structural Relations and Electronic Structure´. **2010**, 636, 1821-1826	5
1845	BaNi2Ge and Ca4Ni4Ge3 □Two layered Structures with $rm ^2_infty$[Ni2Ge] and, $rm ^2_infty$[Ni4Ge3] Networks´. **2010**, 636, 1870-1879	9
1844	Methodologies to analyze surface bonding properties using parametric and density functional methods. **2010**, 110, 743-754	4
1843	New quaternary complex borides, Ti9M2Ru18B8 (Cr, Mn, Co, Ni, Cu, Zn): synthesis, crystal structure and bonding analysis. **2010**, 225, 180-186	12
1842	Variation of equation of state parameters in the Mg2(Si(1-x)Sn(x)) alloys. **2010**, 22, 352204	8
1841	Ternary nitride GaFe(3)N: an experimental and quantum-theoretical study. **2010**, 49, 10148-55	24
1840	New noncentrosymmetric tellurite phosphate material: synthesis, characterization, and calculations of Te2O(PO4)2. **2010**, 49, 7028-34	79
1839	Isolated infinity1[ZnPn2]4- chains in the Zintl phases Ba2ZnPn2 (Pn = As, Sb, Bi)--synthesis, structure, and bonding. **2010**, 49, 5173-9	51
1838	Ru9Zn7Sb8: a structure with a 2 □2 □2 supercell of the half-Heusler phase. **2010**, 49, 10536-42	9

1837	EuAgxAl11− with the BaHg11-Type Structure: Composition, Coloring, and Competition with the BaCd11-Type Structure. **2010**, 22, 1798-1806	13
1836	K(23)Au(12)Sn(9)--an intermetallic compound containing a large gold-tin cluster: synthesis, structure, and bonding. **2010**, 49, 1503-9	7
1835	Structure change via partial Se/Te substitution: crystal structure and physical properties of the telluride Ba(2)Cu(4-x)Te(5) in contrast to the selenide-telluride Ba(2)Cu(4-x)Se(y)Te(5-y). **2010**, 49, 6518-24	16
1834	La4LiAuO8 and La2BaPdO5: comparing two highly stable d8 square-planar oxides. **2010**, 49, 4670-80	16
1833	Rhombohedrally distorted □brasses Cr(1-x)Fe(x)Ga. **2010**, 49, 11505-15	9
1832	Crystal Structure and Physical Properties of the New Antimonide Hf3Cu2Ge3.58Sb1.42. **2010**, 22, 6433-6437	5
1831	Structural and magnetic characteristics of Gd5Ga(x)Si(4-x). **2010**, 49, 4586-93	17
1830	Multiple nonstoichiometric phases with discrete composition ranges in the CaAu5-CaAu4Bi-BiAu2 system. A case study of the chemistry of spinodal decomposition. **2010**, 132, 5662-71	8
1829	Contrasts in structural and bonding representations among polar intermetallic compounds. Strongly differentiated Hamilton populations for three related condensed cluster halides of the rare-earth elements. **2010**, 49, 9949-57	16
1828	BaGa2Pn2 (Pn = P, As): new semiconducting phosphides and arsenides with layered structures. **2010**, 49, 7935-40	34
1827	Orientationally disordered H2 in the high-pressure van der Waals compound SiH4(H2)2. **2010**, 82,	20
1826	Nature of N-N bonding within high-pressure noble-metal pernitrides and the prediction of lanthanum pernitride. **2010**, 132, 2421-9	70
1825	Mixed cations and structural complexity in (Eu(1-x)Ca(x))(4)In(3)Ge(4) and (Eu(1-x)Ca(x))(3)In(2)Ge(3)--the first two members of the homologous series A(2[n+m])In(2n+m)Ge(2[n+m]) (n, m = 1, 2, ...infinity; A = Ca, Sr, Ba, Eu, or Yb). **2010**, 49, 1773-83	26
1824	Sn-flux syntheses, characterizations and bonding analyses of OsB and TiB2. **2010**, 489, 339-342	16
1823	Ternary arsenides Zr(SixAs1−)As with PbCl2-type (0 ≤ x ≤ 0.4) and PbFCl-type (x = 0.6) structures. **2010**, 492, 19-25	5
1822	Different clusters within the Ba4M4−A2Te9 (M=Cu, Ag, Au; A=Si, Ge) series: Crystal structures and transport properties. **2010**, 493, 70-76	7
1821	First-principles prediction on the high-pressure structures of transition metal diborides (TMB2, TM = Sc, Ti, Y, Zr). **2010**, 49, 6859-64	29
1820	Phase change materials and their application to nonvolatile memories. **2010**, 110, 240-67	613

1819	Synthesis, crystal and electronic structures of the new quaternary phases A5Cd2Sb5F (A = Sr, Ba, Eu), and Ba5Cd2Sb5O(x) (0.5. **2010**, 39, 11335-43	14
1818	Novel condensation of Au-centered trigonal prisms in rare-earth-metal-rich tellurides: Er7Au2Te2 and Lu7Au2Te2. **2010**, 39, 6074-9	11
1817	Crystal structure and physical properties of the new silicide Hf4CuSi4 with planar CuSi4 rectangles. **2010**, 20, 4356	1
1816	Synthesis, crystallographic and theoretical studies of the new Zintl phases Ba2Cd2Pn3 (Pn = As, Sb), and the solid solutions (Ba(1-x)Sr(x))2Cd2Sb3 and Ba2Cd2(Sb(1-x)As(x))3. **2010**, 39, 1063-70	60
1815	Syntheses, crystal structures and thermoelectric properties of two new thallium tellurides: Tl4ZrTe4 and Tl4HfTe4. **2010**, 20, 7485	27
1814	Octahedral niobium cluster-based solid state halides and oxyhalides: effects of the cluster condensation via an oxygen ligand on electronic and magnetic properties. **2011**, 35, 2245	18
1813	Relativistic effects and gold site distributions: synthesis, structure, and bonding in a polar intermetallic Na6Cd16Au7. **2011**, 50, 7033-9	15
1812	Complete titanium substitution by boron in a tetragonal prism: exploring the complex boride series Ti(3-x)Ru(5-y)Ir(y)B(2+x) (0 x 1 and 1 2011, 50, 3332-41	18
1811	P2(2-) and P(3-) units in the [Rh8P9] polyanion of La4Rh8P9. **2011**, 50, 3044-51	4
1810	Revisiting the Zintl-Klemm concept: alkali metal trielides. **2011**, 50, 7625-36	29
1809	Synthesis, structure, and bonding of BaTl4. Size effects on encapsulation of cations in electron-poor metal networks. **2011**, 50, 238-44	3
1808	Ca14Au46Sn5: a "colored" Gd14Ag51-type structure containing columns of well-differentiated hexagonal gold stars. **2011**, 50, 1808-15	19
1807	Synthesis, characterization, and structure-property relationships in two new polar oxides: Zn2(MoO4)(SeO3) and Zn2(MoO4)(TeO3). **2011**, 50, 5215-22	64
1806	Zn13(CrxAl1)27 (x = 0.34 0.37): a new intermetallic phase containing icosahedra as building units. **2011**, 226, 557-567	4
1805	Crystal structures, electronic structures, and physical properties of Tl4MQ4 (M = Zr or Hf; Q = S or Se). **2011**, 50, 245-9	13
1804	Scaffolding, ladders, chains, and rare ferrimagnetism in intermetallic borides: electronic structure calculations and magnetic ordering. **2011**, 133, 6832-40	20
1803	Synthesis, structure, and bonding of orthorhombic R5Au2Te2 (R = Lu, Ho, Dy, Y). Electronic structure of the binary parent valence compound Eu5As4. **2011**, 50, 10949-55	11
1802	Chemical pressure and rare-earth orbital contributions in mixed rare-earth silicides La(5-x)Y(x)Si4 (0 x 5). **2011**, 50, 12714-23	14

1801	Crystal orbital Hamilton population (COHP) analysis as projected from plane-wave basis sets. **2011**, 115, 5461-6	1057
1800	A Guided Tour Through Modern Charge Density Analysis. **2011**, 1-78	2
1799	Ternary intermetallics Hf13.0Ni40.8Ga30.9 and Zr13.0Ni40.6Ga31.0. **2011**, 19, 1635-1641	
1798	Structural variations in the ternary system HfAl2−xCux (x´=´0.2−1.0). **2011**, 19, 1849-1856	
1797	Electronic properties of oxides: Chemical and theoretical approaches. **2011**, 39, 70-95	53
1796	Pressure-driven changes in electronic structure of BiCoO3. **2011**, 83,	16
1795	Density functional analysis of the electronic structure of Cs9InO4:Evidence for the presence of a Cs−anion. **2011**, 226, 553-556	3
1794	Electronic Structure of Solids. **2011**,	
1793	Calculation of the electronic structure of delafossite AgTaN2 from first principles. **2011**, 119, 663-666	6
1792	Crystal and electronic structure study of AgPd3Se. **2011**, 184, 2794-2798	7
1791	YbOs4Sb12 Filled Skutterudite: Its Electronic Properties. **2011**, 24, 1957-1962	
1790	Influence of chemical composition and magnetic effects on the elastic properties of fcc Fe−Mn alloys. **2011**, 59, 1493-1501	32
1789	Synthesis, Crystal Structures and Properties of the Zintl Phases Sr2ZnP2, Sr2ZnAs2, A2ZnSb2 and A2ZnBi2 (A = Sr and Eu). **2011**, 637, 2018-2025	39
1788	On the Solid Solution Series Er15[(Fe1−xRux)8C25]: Site Preference for Substitution in the Range 0 ⩽x⩽0.625?. **2011**, 637, 1687-1692	1
1787	HfSb2−xTex: The Second New Compound on the Quasi-Binary Section HfSb2-HfTe2 with Different Sb−Sb Interactions. **2011**, 637, 2033-2038	0
1786	Metastable Bi8Ni8S by Reductive Pseudomorphosis of Bi8Ni8SI2. **2011**, 637, 2026-2032	15
1785	Synthesis, Structure and Chemical Bonding of Ba2Ni5Ge4 □An Intermetallic Compound with a New Two-dimensional rm^2_infty[Ni5Ge4] Structural Motif. **2011**, 637, 2000-2006	2
1784	Carbon-Induced Ordering in Manganese-Rich Austenite □A Density-Functional Total-Energy and Chemical-Bonding Study. **2011**, 82, 101-107	38

1783	Gallium Pnictides of the Alkaline Earth Metals, Synthesized by Means of the Flux Method: Crystal Structures and Properties of CaGa2Pn2, SrGa2As2, Ba2Ga5As5, and Ba4Ga5Pn8 (Pn = P or As). **2011**, 2011, 4025-4036	17
1782	Synthesis, Structure, and Thermoelectric Properties of Barium Copper Polychalcogenides with Chalcogen-Centered Cu Clusters and Te22− Dumbbells. **2011**, 2011, 4037-4042	16
1781	Revisiting the Zintl–Klemm Concept: A2AuBi (A = Li or Na). **2011**, 2011, 3989-3998	11
1780	Mg1−yScyZn2: Limited Sc/Mg Alloying between Laves Phase MgZn2 and ScZn2 − What Drives ScZn2 into a High-Pressure Phase?. **2011**, 2011, 3931-3935	4
1779	Complex Intermetallic Compounds: CaNi5Ge3, Ca15Ni68Ge37, and Ca7Ni49Ge22 − Three Multifaceted Ni-Ge Framework Structures Combining the Structural Motifs of Ni3Ge and CaNi2Ge2. **2011**, 2011, 4012-4024	5
1778	Crystal Structure, Charge Transport, and Magnetic Properties of MnSb2Se4. **2011**, 2011, 3969-3977	28
1777	Ein metastabiles Metall mit lokaler dekagonaler Symmetrie aus einer Niedertemperatur-Pseudomorphose. **2011**, 123, 6302-6304	16
1776	A metastable metal with decagonal local symmetry obtained by low-temperature pseudomorphosis. **2011**, 50, 6178-80	17
1775	A new phase in the binary iron nitrogen system?--The prediction of iron pernitride, FeN2. **2011**, 17, 2598-603	34
1774	Synthesis, crystal and electronic structures, and magnetic properties of LiLn9Mo16O35 (Ln = La, Ce, Pr, and Nd) compounds containing the original cluster Mo16O36. **2011**, 17, 13806-13	2
1773	Syntheses, and crystal and electronic structures of the new Zintl phases Na2ACdSb2 and K2ACdSb2 (A=Ca, Sr, Ba, Eu, Yb): Structural relationship with Yb2CdSb2 and the solid solutions Sr2−xAxCdSb2, Ba2−xAxCdSb2 and Eu2−xYbxCdSb2. **2011**, 184, 432-440	33
1772	Synthesis, crystal and electronic structure, and physical properties of the new lanthanum copper telluride La3Cu5Te7. **2011**, 184, 516-522	9
1771	Elastic properties of Ca-based metallic glasses predicted by first-principles simulations. **2011**, 84,	19
1770	Quantum transport in chemically modified two-dimensional graphene: From minimal conductivity to Anderson localization. **2011**, 84,	66
1769	Thermoelectric Properties of New Thallium Tellurides. **2011**, 1309, 23	1
1768	Quantitative Advances in the Zintl–Klemm Formalism. **2011**, 1-55	41
1767	Noninvasive embedding of single Co atoms in Ge(111)2 × 1 surfaces. **2012**, 85,	13
1766	Multinary selenides with unusual coordination environment of bismuth. **2012**, 51, 13328-33	5

1765	Generalization of Natural Bond Orbital Analysis to Periodic Systems: Applications to Solids and Surfaces via Plane-Wave Density Functional Theory. **2012**, 8, 1902-11	140
1764	LaSrVMoO6: A case study for A-site covalency-driven local cationic order in double perovskites. **2012**, 86,	5
1763	Hydrophilicity control of visible-light hydrogen evolution and dynamics of the charge-separated state in dye/TiO2/Pt hybrid systems. **2012**, 18, 15368-81	47
1762	Atomic site preferences and its effect on magnetic structure in the intermetallic borides M2Fe(Ru0.8T0.2)5B2 (M=Sc, Ti, Zr; T=Ru, Rh, Ir). **2012**, 196, 168-174	7
1761	Crystal structure and chemical bonding of novel Li-containing polar intermetallic compound La11Li12Ge16. **2012**, 196, 543-549	5
1760	Synthesis of alkaline earth diazenides M(AE)N2 (M(AE) = Ca, Sr, Ba) by controlled thermal decomposition of azides under high pressure. **2012**, 51, 2366-73	41
1759	Chemical modeling of mixed occupations and site preferences in anisotropic crystal structures: case of complex intermetallic borides. **2012**, 51, 5677-85	14
1758	Two homologous intermetallic phases in the Na-Au-Zn system with sodium bound in unusual paired sites within 1D tunnels. **2012**, 51, 9395-402	13
1757	Synthesis, crystal structure, chemical bonding, and physical properties of the ternary Na/Mg stannide Na2MgSn. **2012**, 51, 4810-6	14
1756	Structural phase transitions in SrRh2As2. **2012**, 85,	15
1755	Gold derivatives of eight rare-earth-metal-rich tellurides: monoclinic R7Au2Te2 and orthorhombic R6AuTe2 types. **2012**, 51, 3548-56	18
1754	Four polyanionic compounds in the K□Au□a system: a case study in exploratory synthesis and of the art of structural analysis. **2012**, 51, 1695-702	32
1753	Gd13Fe10C13: indications of Fe-Fe multiple bonding emerging from chemical frustration. **2012**, 134, 10361-4	12
1752	The □ model of acids and bases: extending the Lewis theory to intermetallics. **2012**, 51, 4250-64	12
1751	New ternary germanides La4Mg5Ge6 and La4Mg7Ge6: crystal structure and chemical bonding. **2012**, 51, 207-14	23
1750	Synthesis, structure, chemical bonding, and magnetism of the series RELiGe2 (RE = La-Nd, Sm, Eu). **2012**, 51, 620-8	27
1749	Validation of interstitial iron and consequences of nonstoichiometry in mackinawite (Fe(1+x)S). **2012**, 116, 2234-43	14
1748	BaAu(x)Zn(13-x): electron-poor cubic NaZn13-type intermetallic and its ordered tetragonal variant. **2012**, 51, 2247-53	16

1747	Closely related rare-earth metal germanides RE2Li2Ge3 and RE3Li4Ge4 (RE = La-Nd, Sm): synthesis, crystal chemistry, and magnetic properties. **2012**, 51, 3119-29	26
1746	Three alkali-metal-gold-gallium systems. Ternary tunnel structures and some problems with poorly ordered cations. **2012**, 51, 7711-21	34
1745	Crystal structure and physical properties of the new one-dimensional metal Ba2Cu(7-x)Te6. **2012**, 51, 5299-304	6
1744	Detailed insights into the structural properties and oxygen-pathways in orthorhombic Ba0.5Sr0.5Co0.8Fe0.2O3 by electronic-structure theory. **2012**, 222-223, 53-58	19
1743	Unique geometric and electronic structure of CO adsorbed on Ge(100): A DFT study. **2012**, 606, 784-790	6
1742	Investigation of the bonding of SiHn and CHn (n=1,2,3) on Cu(111) using DFT. **2012**, 258, 7546-7551	6
1741	Eleven new compounds in the RE Cd Ge systems (RE=Pr, Nd, Sm, Gd Yb; Y): Crystal chemistry of the RE2CdGe2 series. **2012**, 192, 16-22	11
1740	The complex metal-rich boride Ti1+xRh2+yIr3B3 (x=0.68, y=1.06) with a new structure type containing B4 zigzag fragments: Synthesis, crystal chemistry and theoretical calculations. **2012**, 192, 113-119	18
1739	DFT-chemical pressure analysis: visualizing the role of atomic size in shaping the structures of inorganic materials. **2012**, 134, 5991-9	39
1738	Synthesis and Crystallochemical Characterisation of the Intermetallic Phases La(AgxMg1)12 (0.11 x 0.21), LaAg4+xMg2 (0.15 x 1.05) and LaAg2+xMg2 (0 2012, 2012, 4811-4821	15
1737	Synthesis, Structure, and Bonding Analysis of the Polar Intermetallic Phase Ca2Pt2Cd. **2012**, 638, 1963-1969	10
1736	The Prolific {ZR6}X12R and {ZR6}X10 Structure Types with Isolated Endohedrally Stabilized (Z) Rare-Earth Metal (R) Cluster Halide (X) Complexes. **2012**, 638, 1922-1931	13
1735	Study of the antiferromagnetism of Mn5Si3: an inverse magnetocaloric effect material. **2012**, 22, 15275	29
1734	On the nature of Ge-Pb bonding in the solid state. Synthesis, structural characterization, and electronic structures of two unprecedented germanide-plumbides. **2012**, 134, 12708-16	6
1733	Synthesis of BiRh Nanoplates with Superior Catalytic Performance in the Semihydrogenation of Acetylene. **2012**, 24, 1639-1644	40
1732	Synthesis, Crystal and Electronic Structures, and Thermoelectric Properties of the Novel Cluster Compound Ag3In2Mo15Se19. **2012**, 24, 2899-2908	46
1731	Spatially Resolved Electronic Alterations As Seen by in Situ195Pt and 13CO NMR in [email´protected] and [email´protected] Core Shell Nanoparticles. **2012**, 116, 26480-26486	15
1730	Chemical Bonding and Hybridization in 5p Binary Oxide. **2012**, 116, 24248-24254	15

1729	Ca10Pt7Tt3 (Tt = Si, Ge): new platinide phases featuring electron-rich 4c-6e bonded [Pt7Tt3]20- intermetalloid clusters. **2012**, 51, 11980-5	10
1728	Identifying a structural preference in reduced rare-earth metal halides by combining experimental and computational techniques. **2012**, 51, 11356-64	20
1727	Nb3Ru5B2 The First Fully Characterized Ternary Phase in the Nb-Ru-B System: Synthesis, Crystal Structure, and Bonding Analysis. **2012**, 638, 49-52	13
1726	Polymorphism of Li2Zn3. **2012**, 68, 34-9	10
1725	Crystal Structure and Electronic Structure of Red SnO. **2012**, 638, 1970-1975	20
1724	Formation of nets of corner-shared bicapped gold squares in SrAu3Ge: how a BaAl4-type derivative reconciles fewer valence electrons and the origin of its uniaxial negative thermal expansion. **2012**, 134, 4877-84	15
1723	Planarer B6-Ring in der Festkperverbindung Ti7Rh4Ir2B8. **2012**, 124, 1734-1737	17
1722	Synthesis, crystal chemistry, and magnetic properties of RE7Li8Ge10 and RE11Li12Ge16 (RE = La-Nd, Sm): new members of the [REGe2](n)[RELi2Ge](m) homologous series. **2012**, 51, 6821-9	20
1721	Dehydration kinetics and crystal water dynamics of carbamazepine dihydrate. **2012**, 29, 1143-57	20
1720	Mechanical properties and chemical bonding of the OsB system: A first-principles study. **2012**, 60, 4208-4217	31
1719	Synthesis and structural characterization of the ternary Zintl phases AE3Al2Pn4 and AE3Ga2Pn4 (AE=Ca, Sr, Ba, Eu; Pn=P, As). **2012**, 188, 59-65	32
1718	Ca2NiSn2 A Polymorphic Intermetallic Phase: Atomic and Electronic Structure as well as a Topological Description of the Phase Transition by a Sigmatropic-Type Rearrangement of Ni and Sn Atoms. **2012**, 2012, 987-997	5
1717	All-boron planar B6 ring in the solid-state phase Ti7Rh4Ir2B8. **2012**, 51, 1702-5	54
1716	Correlations between chemical bonding and magnetic exchange interactions: synthesis, crystal structures, and magnetic properties of the new family RE2AlGe2 (RE = Tb-Tm, Lu). **2013**, 52, 5307-15	10
1715	Synthesis, crystal and electronic structures and magnetic properties of Li2SnMo3O8: A novel reduced molybdenum oxide containing Mo3O13 cluster units. **2013**, 201, 312-316	3
1714	Transition-Metal Pnictides. **2013**, 111-135	3
1713	Crystal Structure and Bonding in Intermetallic Compounds. **2013**, 359-373	22
1712	Metal-Rich Compounds of the d-Metals. **2013**, 311-357	6

1711	Computational Methods for Solids. **2013**, 59-87	2
1710	Theoretical analysis of the structure and bonding in electron-rich edge-bridged octahedral tungsten chloride clusters. **2013**, 19, 150-155	2
1709	Synthesis and single-crystal structure determination of the zinc nitride halides Zn2NX (X=Cl, Br, I). **2013**, 203, 31-36	7
1708	Unprecedented electron-poor octahedral Ta(6) clusters in a solid-state compound: synthesis, characterisations and theoretical investigations of Cs(2)BaTa(6)Br(15)O(3). **2013**, 19, 12711-9	11
1707	High-pressure synthesis and characterization of Li2Ca3[N2]3--an uncommon metallic diazenide with [N2]2- ions. **2013**, 135, 16668-79	17
1706	Probing actinide electronic structure through pu cluster calculations. **2013**, 113, 1957-1965	14
1705	Polyclusters and substitution effects in the Na-Au-Ga system: remarkable sodium bonding characteristics in polar intermetallics. **2013**, 52, 12502-10	17
1704	Synthesis and structural characterization of RE7Zn21Tt2 (RE = La-Nd; Tt = Ge, Sn, and Pb): new structure type among the polar intermetallic phases. **2013**, 52, 12731-40	8
1703	Gold network structures in rhombohedral and monoclinic Sr2Au6(Au,T)3 (T = Zn, Ga). A transition via relaxation. **2013**, 52, 13623-30	20
1702	Ab initio studies of ternary semiconductor BeB2C2. **2013**, 68, 174-180	9
1701	Adhesion of the TiN/Fe interface with point defects from first principles. **2013**, 113, 014905	9
1700	Phosphide oxides RE2AuP2O (RE = La, Ce, Pr, Nd): synthesis, structure, chemical bonding, magnetism, and 31P and 139La solid state NMR. **2013**, 52, 2094-102	12
1699	Analytic projection from plane-wave and PAW wavefunctions and application to chemical-bonding analysis in solids. **2013**, 34, 2557-67	790
1698	Caesium in high oxidation states and as a p-block element. **2013**, 5, 846-52	142
1697	Structural and relative stabilities, electronic properties and possible reactive routing of osmium and ruthenium borides from first-principles calculations. **2013**, 42, 7041-50	27
1696	Determination of a new structure type in the Sc-Fe-Ge-Sn system. **2013**, 546, 300-306	0
1695	Ca2Pd3Ge, a new fully ordered ternary Laves phase structure. **2013**, 197, 312-316	19
1694	Y3MnAu5: three distinctive d-metal functions in an intergrown cluster phase. **2013**, 135, 910-7	9

1693	Electronic structure, chemical bonding and magnetism of the metal-rich borides MRh6B3 (M = Cr, Mn, Fe, Co, Ni) with Th7Fe3-type structure: A density functional theory study. **2013**, 17, 14-20	6
1692	Combined effect of chemical pressure and valence electron concentration through the electron-deficient Li substitution on the RE4LiGe4 (RE=La, Ce, Pr, and Sm) system. **2013**, 205, 10-20	15
1691	Na8Au9.8(4)Ga7.2 and Na17Au5.87(2)Ga46.63: The diversity of pseudo 5-fold symmetries in the Na–Au–Ga system. **2013**, 207, 21-28	18
1690	Electronic and atomic structure of Co/Ge nanoislands on the Ge(111) surface. **2013**, 88,	5
1689	Rare earth–zinc–germanides RE4Zn5Ge6 (RE = Y, Dy, Ho, Er) and RE5Zn4Ge6 (RE = Er, Tm, Lu). **2013**, 38, 36-43	5
1688	Synthesis, crystal and electronic structures of the new Zintl phases Ba3Al3Pn5 (Pn = P, As) and Ba3Ga3P5. **2013**, 52, 499-505	9
1687	Systematic study on the electronic structure and mechanical properties of X2BC (X = Mo, Ti, V, Zr, Nb, Hf, Ta and W). **2013**, 25, 045501	35
1686	Chemistry on the Surface. **2013**, 691-734	
1685	High hydrogen content super-lightweight intermetallics from the Li–Mg–Si system. **2013**, 38, 5724-5737	14
1684	Synthesis, structure and chemical bonding of CaFe2–xRhxSi2 (x=0, 1.32, and 2) and SrCo2Si2. **2013**, 203, 232-239	9
1683	Does the real ReN2 have the MoS2 structure?. **2013**, 15, 183-7	20
1682	Disorder-order structural transformation in electron-poor Sr3Au8Sn3 driven by chemical bonding optimization. **2013**, 52, 6603-9	6
1681	First-Principles Elucidation of Atomic Size Effects Using DFT-Chemical Pressure Analysis: Origins of Ca36Sn23's Long-Period Superstructure. **2013**, 9, 3170-80	25
1680	BaAu2P4: layered zintl polyphosphide with infinite [1](P)[1] chains. **2013**, 52, 7061-7	30
1679	Nb2OsB2, with a new twofold superstructure of the U3Si2 type: Synthesis, crystal chemistry and chemical bonding. **2013**, 203, 304-309	15
1678	Hexagonal-diamond-like gold lattices, Ba and (Au,T)3 interstitials, and delocalized bonding in a family of intermetallic phases Ba2Au6(Au,T)3 (T = Zn, Cd, Ga, In, or Sn). **2013**, 135, 11023-31	27
1677	Magnetic ordering in tetragonal 3d metal arsenides M2As (M = Cr, Mn, Fe): an ab initio investigation. **2013**, 52, 3013-21	4
1676	The Y5–Mg24+x(1.08(4)–1.30(1)) series and a ternary derivative Ce6.9Y12.5(7)Mg92.2: A comparison of their crystal and electronic structures. **2013**, 204, 170-177	8

1675	Review on cerium intermetallic compounds: A bird's eye outlook through DFT. **2013**, 41, 55-85	25
1674	From one to three dimensions: corrugated [1)[NiGe] ribbons as a building block in alkaline earth metal Ae/Ni/Ge phases with crystal structure and chemical bonding in AeNiGe (Ae = Mg, Sr, Ba). **2013**, 52, 6905-15	8
1673	A ferrimagnetic Zintl phase Pr4MnSb9: synthesis, structure, and physical properties. **2013**, 52, 7441-7	7
1672	Ab initio investigations of the electronic structures and chemical bonding in LiCo6P4 and Li2Co12P7. **2013**, 202, 227-233	4
1671	Structural acid-base chemistry in the metallic state: how [3-neutralization drives interfaces and helices in Ti21Mn25. **2013**, 52, 8349-59	8
1670	New polar intermetallic phases RE2Zn5Tt (RE = La-Nd; Tt = Sn and Pb): synthesis, structure, chemical bonding, and magnetic properties. **2013**, 52, 9102-10	8
1669	Cluster chemistry in electron-poor Ae-Pt-Cd systems (Ae = Ca, Sr, Ba): (Sr,Ba)Pt2Cd4, Ca6Pt8Cd16, and its known antitype Er6Pd16Sb8. **2013**, 52, 2697-704	13
1668	Substantial Cd-Cd bonding in Ca6PtCd11: a condensed intermetallic phase built of pentagonal Cd7 and rectangular Cd4/2Pt pyramids. **2013**, 52, 10112-8	9
1667	Ten-Million-Atom Electronic Structure Calculations on the K Computer with a Massively Parallel Order-NTheory. **2013**, 82, 023710	6
1666	A density-functional theory study of tip electronic structures in scanning tunneling microscopy. **2013**, 24, 105201	6
1665	Gold[Structural Versatility within Complex Intermetallics: From Hume-Rothery to Zintl and even Quasicrystals. **2013**, 1517, 1	2
1664	First-Principles Study on Energy Property and Stability of Y3Al5O12 Crystal. **2013**, 634-638, 2531-2536	
1663	V1+xNb1[IrB2 (x [0.1), The First Quaternary Metal-Rich ŕBoride Adopting The Mo2IrB2-Type Structure: Synthesis, Crystal and Electronic Structure and Bonding Analysis. **2013**, 639, 319-325	2
1662	A first-principles study on defect association and oxygen ion migration of Sm3+ and Gd3+ co-doped ceria. **2013**, 25, 225401	17
1661	Nanosession: Phase Change Memories. **2013**, 163-176	
1660	Synthesis and crystal chemistry of new ternary pnictides containing lithium--adding structural complexity one step at a time. **2014**, 43, 16889-901	14
1659	Synthesis and Characterization of the Ternary Telluroargentate K4[Ag18Te11]. **2014**, 640, 2939-2944	7
1658	Adsorption of ammonia at GaN(0001) surface in the mixed ammonia/hydrogen ambient - a summary of ab initio data. **2014**, 4, 117109	22

1657	Site preference and magnetic orderings in the intermetallic boride series M 1.5 Rh 5.5 B 3 (M = Cr, Mn, Fe, Co, Ni) from first principles DFT calculations. **2014**, 92, 416-421	3
1656	First-principles calculation of elastic moduli of early-late transition metal alloys. **2014**, 89,	7
1655	Nanosecond quantum molecular dynamics simulations of the lithium superionic conductor Li4□Ge1□PxS4. **2014**, 90,	16
1654	Structural, electronic, and optical properties of GaInO3: A hybrid density functional study. **2014**, 115, 043708	29
1653	Complex Polyanionic Nets in RbAu4.01(2)Ga8.64(5) and CsAu5Ga9: The Role of Cations in the Formation of New Polar Intermetallics. **2014**, 640, 790-796	8
1652	Electronic and bonding analysis of hardness in pyrite-type transition-metal pernitrides. **2014**, 90,	70
1651	Fermi level pinning and the charge transfer contribution to the energy of adsorption at semiconducting surfaces. **2014**, 115, 043529	18
1650	A novel stable binary BeB□phase [corrected]. **2014**, 4, 6993	21
1649	Bonding nature of local structural motifs in amorphous GeTe. **2014**, 53, 10817-20	102
1648	Experimental and Theoretical Investigations of the Ternary Boride NbRuB with a Layerlike Structure Type. **2014**, 2014, 1381-1388	14
1647	First-principles study of bismuth films at transition-metal grain boundaries. **2014**, 90,	14
1646	Structural and Thermal Characterization of the Incorporation of Lithium into ZnO. **2014**, 2014, 925-931	5
1645	Bindungseigenschaften lokaler Strukturmotive in amorphem GeTe. **2014**, 126, 10993-10997	3
1644	Penta-lanthanum zinc diplumbide, La5Zn1-x Pb2+x (x ? 0.6). **2014**, 70, i2-i3	3
1643	Toward a better understanding of the magnetocaloric effect: An experimental and theoretical study of MnFe4Si3. **2014**, 216, 56-64	11
1642	Structural distortion and band gap opening of hard MnB4 in comparison with CrB4 and FeB4. **2014**, 213, 52-56	24
1641	Bonding in intermetallics may be deceptive □The case of the new type structure Au2InGa2. **2014**, 46, 40-44	6
1640	The layered antimonides RELi3Sb2 (RE=Ce□Nd, Sm, Gd□Ho). Filled derivatives of the CaAl2Si2 structure type. **2014**, 210, 89-95	13

1639	Atomistic model of fluorescence intermittency of colloidal quantum dots. **2014**, 112, 157401	65
1638	Taking Advantage of Gold Electronegativity in R4Mn3Au10+x (R = Gd or Y; 0.2 x 1). **2014**, 26, 3209-3218	8
1637	General aspects of the vapor growth of semiconductor crystals A study based on DFT simulations of the NH3/NH2 covered GaN(0001) surface in hydrogen ambient. **2014**, 390, 71-79	11
1636	Self-assembled nano- to micron-size fibers from molten R11Ni4In9 intermetallics. **2014**, 73, 27-36	8
1635	Binary Lithium Indides Li22In8+x (x = 0.1), Li11In4+x (x = 1.05), and Li10In2+x (x = 1.59) with Clusters. **2014**, 2014, 2053-2064	3
1634	The role of equilibrium volume and magnetism on the stability of iron phases at high pressures. **2014**, 26, 046001	4
1633	The RELixSn2 (RE=La Nd, Sm, and Gd; 0 . **2014**, 211, 95-105	11
1632	Ba3TM2Se9 (TM = Nb, Ta): synthesis and characterization of new polyselenides. **2014**, 53, 80-4	1
1631	Thermochemical Ranking and Dynamic Stability of TeO2 Polymorphs from Ab Initio Theory. **2014**, 14, 871-878	29
1630	Electronic structure of ternary rhodium hydrides with lithium and magnesium. **2014**, 53, 1135-43	4
1629	X-ray characterization, electronic band structure, and thermoelectric properties of the cluster compound Ag2Tl2Mo9Se11. **2014**, 53, 11699-709	40
1628	New Lithium-Containing Pnictides with 1-D Infinite Chains of Supertetrahedral Clusters: Synthesis, Crystal and Electronic Structure of Ba4Li2Cd3Pn6 (Pn = P, As and Sb). **2014**, 2014, 5113-5124	11
1627	Role of Interchain Interaction in Determining the Band Gap of Trigonal Selenium: A Density Functional Theory Study with a Linear Combination of Bloch Orbitals. **2014**, 118, 19294-19307	5
1626	Conjugation in Gd13Fe10C13 and its oxycarbide: unexpected connections between complex carbides and simple organic molecules. **2014**, 136, 12073-84	9
1625	Novel Si Networks in the Ca/Si Phase Diagram under Pressure. **2014**, 118, 25167-25175	12
1624	First-Principles Studies of Lithium Adsorption and Diffusion on Graphene with Grain Boundaries. **2014**, 118, 28055-28062	62
1623	Spin polarization gives rise to Cu precipitation in Fe-matrix. **2014**, 16, 7222-30	8
1622	Magnetically stabilized Fe8(4-S)6S8 clusters in Ba6Fe25S27. **2014**, 43, 14612-24	6

1621	Turning gold into "diamond": a family of hexagonal diamond-type Au-frameworks interconnected by triangular clusters in the Sr-Al-Au system. **2014**, 136, 3108-17	25
1620	The hydrogen adsorption on Zr-decorated LiB (001): A DFT study. **2014**, 110, 62-68	11
1619	Pressure-stabilized lithium caesides with caesium anions beyond the -1 state. **2014**, 5, 4861	34
1618	Synthesis, crystal structure, and magnetic properties of novel intermetallic compounds R2Co2SiC (R = Pr, Nd). **2014**, 53, 6141-8	7
1617	Influence of the Ba2+/Sr2+ content and oxygen vacancies on the stability of cubic Ba(x)Sr(1-x)Co(0.75)Fe(0.25)O(3-□). **2014**, 16, 1333-8	7
1616	On a new FeOF polymorph: Synthesis and stability. **2014**, 38, 55-61	4
1615	Valence state driven site preference in the quaternary compound Ca5MgAgGe5: an electron-deficient phase with optimized bonding. **2014**, 53, 4724-32	8
1614	Silicon monoxide at 1 atm and elevated pressures: crystalline or amorphous?. **2014**, 136, 3410-23	20
1613	Pronounced matrix effect in YbMo2Al4-type Ca(AuxZn2□)Au4 (x=0.09□.89). **2014**, 218, 103-108	8
1612	Layered compounds BaM2Ge4Ch6 (M = Rh, Ir and Ch = S, Se) with pyrite-type building blocks and Ge-Ch heteromolecule-like anions. **2014**, 53, 5684-91	3
1611	Covalency of hydrogen bonds in solids revisited. **2014**, 50, 11547-9	39
1610	Peierls-distorted monoclinic MnB(4) with a Mn-Mn bond. **2014**, 53, 1684-8	43
1609	Single-crystal growth and size control of three novel polar intermetallics: Eu2.94(2)Ca6.06In8Ge8, Eu3.13(2)Ca5.87In8Ge8, and Sr3.23(3)Ca5.77In8Ge8 with crystal structure, chemical bonding, and magnetism studies. **2014**, 53, 4669-77	6
1608	Atomistic mechanisms of codoping-induced p- to n-type conversion in nitrogen-doped graphene. **2014**, 6, 14911-8	28
1607	Unexpected synergy between magnetic iron chains and stacked B6 rings in Nb6Fe(1-x)Ir(6+x)B8. **2014**, 53, 13174-7	19
1606	Synthesis and theoretical investigations of the solid solution CeRu(1-x)Ni(x)Al (x = 0.1-0.95) showing cerium valence fluctuations. **2014**, 53, 2471-80	14
1605	Isolobal analogies in intermetallics: the reversed approximation MO approach and applications to CrGa4- and Ir3Ge7-type phases. **2014**, 53, 2730-41	41
1604	LiZn(4 - x) (x = 0.825) as a (3 + 1)-dimensional modulated derivative of hexagonal close packing. **2014**, 70, 212-7	10

1603	Experimental and First-Principles Studies of the Ternary Borides Ta3Ru5B2 and M3□Ru5+xB2 (M = Zr, Hf). **2014**, 2014, 3085-3094	8
1602	Electronic, structural and magnetic studies of niobium borides of group 8 transition metals, Nb2MB2 (M=Fe, Ru, Os) from first principles calculations. **2014**, 211, 227-234	12
1601	Progress in Visualizing Atomic Size Effects with DFT-Chemical Pressure Analysis: From Isolated Atoms to Trends in AB5 Intermetallics. **2014**, 10, 3380-92	31
1600	New Co□Pd□Zn □Brasses with Dilute Ferrimagnetism and Co2Zn11 Revisited: Establishing the Synergism between Theory and Experiment. **2014**, 26, 2624-2634	15
1599	Chemical Bonding in Solids. **2014**, 445-476	
1598	DFT study of ammonia desorption from the GaN(0001) surface covered with a NH3/NH2 mixture. **2014**, 403, 105-109	6
1597	Calcium substitution in rare-earth metal germanides with the hexagonal Mn5Si3 structure type. structural characterization of the extended series RE5□CaxGe3 (RE=Rare-earth metal). **2014**, 217, 142-149	1
1596	Symbiosis of Intermetallic and Salt: Rare-Earth Metal Cluster Complexes with Endohedral Transition Metal Atoms. **2014**, 45, 111-178	1
1595	Crystal Structures of Homoleptic Propynyloargentates AI[Ag(C3H3)2] with AI = Ag, Li, Na Solved and Refined from X-ray Powder Diffraction Data. **2014**, 640, 3127-3134	3
1594	Peierls-verzerrtes monoklines MnB4 mit einer Mn-Mn-Bindung. **2014**, 126, 1710-1714	6
1593	Unexpected Synergy between Magnetic Iron Chains and Stacked B6 Rings in Nb6Fe1□Ir6+xB8. **2014**, 126, 13390-13393	6
1592	Impact of Mn on the solution enthalpy of hydrogen in austenitic Fe-Mn alloys: a first-principles study. **2014**, 35, 2239-44	6
1591	Density-functional theory guided advances in phase-change materials and memories. **2015**, 40, 856-869	52
1590	Phonon quarticity induced by changes in phonon-tracked hybridization during lattice expansion and its stabilization of rutile TiO2. **2015**, 92,	12
1589	Pressure-driven formation and stabilization of superconductive chromium hydrides. **2015**, 5, 17764	25
1588	A projection-free method for representing plane-wave DFT results in an atom-centered basis. **2015**, 143, 104109	3
1587	Some Physical Principles of High Temperature Shape Memory Alloys Design. **2015**, 81-82, 207-231	5
1586	Grown from lithium flux, the ErCo5Si(3.17) silicide is a combination of disordered derivatives of the UCo5Si3 and Yb6Co30P19 structure types. **2015**, 71, 506-10	1

1585	Brasses with Spontaneous Magnetization: Atom Site Preferences and Magnetism in the Fe-Zn and Fe-Pd-Zn Phase Spaces. **2015**, 641, 270-278	12
1584	On the Structure and Stability of BaAl4-Type Ordered Derivatives in the Sr-Au-Sn System for the 600 °C Section. **2015**, 641, 375-382	3
1583	Origin of Extraordinary Stability of Square-Planar Carbon Atoms in Surface Carbides of Cobalt and Nickel. **2015**, 127, 5402-5406	4
1582	Synthesis, structure, and properties of SrC(NH)3 , a nitrogen-based carbonate analogue with the trinacria motif. **2015**, 54, 12171-5	7
1581	Synthese, Struktur und Eigenschaften von SrC(NH)3, einem stickstoffbasierten Carbonatanalogon mit Trinacriamotiv. **2015**, 127, 12339-12343	4
1580	Synergistic Geometrical and Electronic Features in the Intermetallic Phases Ca2AgM2, Ca2MgM2, and Ca2GaM2 (M = Pd, Pt). **2015**, 641, 1069-1079	4
1579	CuN3: die übersehene Grundzustandsmodifikation des Kupferazids mit heterographenartigen Schichten. **2015**, 127, 1977-1982	5
1578	Influence of Valence Electron Concentration on Laves Phases: Structures and Phase Stability of Pseudo-Binary MgZn2−xPdx. **2015**, 641, 1486-1494	7
1577	Microscopic Complexity in Phase-Change Materials and its Role for Applications. **2015**, 25, 6343-6359	71
1576	Electron transport in carbon wires in contact with Ag electrodes: a detailed first principles investigation. **2015**, 17, 18413-25	17
1575	Phase stability, chemical bonding and mechanical properties of titanium nitrides: a first-principles study. **2015**, 17, 11763-9	87
1574	Ligand-Hole in [SnI6] Unit and Origin of Band Gap in Photovoltaic Perovskite Variant Cs2SnI6. **2015**, 88, 1250-1255	83
1573	Novel compounds in the Zr-O system, their crystal structures and mechanical properties. **2015**, 17, 17301-10	13
1572	Influence of boron vacancies on phase stability, bonding and structure of MB1−x (M = Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W) with AlB2-type structure. **2015**, 27, 435702	22
1571	Non-stoichiometric compositions arising from synergistic electronic and size effects. Synthesis, crystal chemistry and electronic properties of A14Cd1+xPn11 compounds (0≤x≤0.3; A = Sr, Eu; Pn = As, Sb). **2015**, 3, 10388-10400	14
1570	Chromium substitution effect on structural and electrochemical behavior of Li-Cr-Ni-O oxides. **2015** , 21, 3039-3049	3
1569	Order and disorder in quaternary atomic laminates from first-principles calculations. **2015**, 17, 31810-21	59
1568	Ultrafast palladium diffusion in germanium. **2015**, 3, 3832-3838	12

1567	CuN3: the overlooked ground-state polymorph of copper azide with heterographene-like layers. **2015**, 54, 1954-9	22
1566	Synthesis, structure, and superconductivity in the new-structure-type compound: SrPt6P2. **2015**, 54, 1049-54	9
1565	Vacancy ordering as a driving factor for structural changes in ternary germanides: the new R2Zn(1-x)Ge6 series of polar intermetallics (R = rare-earth metal). **2015**, 54, 2411-24	11
1564	A density-functional study on the electronic and vibrational properties of layered antimony telluride. **2015**, 27, 085402	18
1563	First principles study of the elastic properties of Li2MnSiO4 Sy. **2015**, 3, 5449-5456	21
1562	Synthesis, Structure Determination and Electronic Structure of Magnesium Nitride Chloride, Mg2NCl. **2015**, 641, 266-269	5
1561	Fully and partially Li-stuffed diamond polytypes with Ag-Ge structures: Li2AgGe and Li2.53AgGe2. **2015**, 54, 1152-8	4
1560	Electron counting rules and electronic structure in tetrameric transition-metal (T)-centered rare-Earth (R) cluster complex halides (X). **2015**, 54, 1026-37	14
1559	Linear Metal Chains in Ca2M2X (M = Pd, Pt; X = Al, Ge): Origin of the Pairwise Distortion and Its Role in the Structure Stability. **2015**, 27, 304-315	20
1558	Gold-gold bonding: the key to stabilizing the 19-electron ternary phases LnAuSb (Ln = La-Nd and Sm). **2015**, 137, 1282-9	19
1557	Competition between Direct and Indirect Exchange Couplings in MnFeAs: A First-Principles Investigation. **2015**, 119, 580-589	5
1556	Quaternary pnictides with complex, noncentrosymmetric structures. Synthesis and structural characterization of the new Zintl phases Na11Ca2Al3Sb8, Na4CaGaSb3, and Na15Ca3In5Sb12. **2015**, 54, 1931-9	7
1555	Atomic bonding in the AlLiB14. **2015**, 47, 3-6	1
1554	High-pressure electrides: the chemical nature of interstitial quasiatoms. **2015**, 137, 3631-7	94
1553	Crystal Structure and Chemical Bonding Analysis of BaPtCd2. **2015**, 641, 557-560	6
1552	Twisted Kelvin Cells and Truncated Octahedral Cages in the Crystal Structures of Unconventional Clathrates, AM2P4 (A = Sr, Ba; M = Cu, Ni). **2015**, 27, 4476-4484	40
1551	Synthesis and crystal structure of Ba26B12Si5N27 containing [Si2] dumbbells. **2015**, 230, 390-396	5
1550	Quantum pressure and chemical bonding: Influence of magnetic fields on electron localization. **2015**, 92,	7

1549	Phase diagram, mechanical properties, and electronic structure of Nb-N compounds under pressure. **2015**, 17, 22837-45	20
1548	First-Principles Design and Analysis of an Efficient, Pb-Free Ferroelectric Photovoltaic Absorber Derived from ZnSnO3. **2015**, 27, 5899-5906	16
1547	Vibrational properties and bonding nature of SbSe and their implications for chalcogenide materials. **2015**, 6, 5255-5262	62
1546	Electronic structure and absolute band edge position of tetragonal AgInS2 photocatalyst: A hybrid density functional study. **2015**, 40, 446-452	38
1545	First-principles investigation of the activation of CO2 molecule on TM/Cu (TM = Fe, Co and Ni) surface alloys. **2015**, 353, 902-912	24
1544	Octahedral and trigonal-prismatic coordination preferences in Nb-, Mo-, Ta-, and W-based ABX2 layered oxides, oxynitrides, and nitrides. **2015**, 229, 272-277	11
1543	Compositional dependence of structures of NiTi martensite from first principles. **2015**, 95, 184-191	8
1542	Crystal structure, chemical bonding and magnetism studies for three quinary polar intermetallic compounds in the (Eu(1-x)Ca(x))9In8(Ge(1-y)Sn(y))8 (x = 0.66, y = 0.03) and the (Eu(1-x)Ca(x))3In(Ge(3-y)Sn(1+y)) (x = 0.66, 0.68; y = 0.13, 0.27) phases. **2015**, 16, 9017-36	1
1541	New quaternary arsenide oxides with square planar coordination of gold(I) - structure, (197)Au Mössbauer spectroscopic, XANES and XPS characterization of Nd10Au3As8O10 and Sm10Au3As8O10. **2015**, 44, 5854-66	9
1540	Electronic structure, thermodynamics, and thermoelectric properties of □BaCu 2 S 2 : A first-principles study. **2015**, 103, 105-110	4
1539	New quaternary oxides with both families of second-order Jahn□eller (SOJT) distortive cations: Solid-state synthesis, structure determination, and characterization of YNbTe2O8 and YNbSe2O8. **2015**, 637, 155-161	6
1538	Stabilization of the Ti3Co5B2-type structure for Ti3□i Ru5B2 through Si□i substitution. **2015**, 227, 92-97	1
1537	Wade□ rules and the stability of AunGem clusters. **2015**, 69, 1	3
1536	Origin of extraordinary stability of square-planar carbon atoms in surface carbides of cobalt and nickel. **2015**, 54, 5312-6	55
1535	Influence of chemical bonding and magnetism on elastic properties of the A2MB2 borides (A=Nb, Ta; M=Fe, Ru, Os) from first-principles calculations. **2015**, 104, 52-59	15
1534	Electronic pseudogap-driven formation of new double-perovskite-like borides within the Sc2Ir6-xTxB (T = Pd, Ni; x = 0-6) series. **2015**, 54, 4056-63	6
1533	The low coordination number of nitrogen in hard tungsten nitrides: a first-principles study. **2015**, 17, 13397-402	19
1532	A large family of filled skutterudites stabilized by electron count. **2015**, 6, 6489	38

1531	Origins of contrasting copper coordination geometries in crystalline copper sulfate pentahydrate. **2015**, 17, 31023-9	23
1530	Ba3Pt4Al4-Structure, Properties, and Theoretical and NMR Spectroscopic Investigations of a Complex Platinide Featuring Heterocubane [Pt4Al4] Units. **2015**, 54, 10785-93	18
1529	Gold-rich R3Au7Sn3: establishing the interdependence between electronic features and physical properties. **2015**, 3, 8311-8321	17
1528	A periodic energy decomposition analysis method for the investigation of chemical bonding in extended systems. **2015**, 142, 194105	55
1527	From the Ternary Eu(Au/In)2 and EuAu4(Au/In)2 with Remarkable Au/In Distributions to a New Structure Type: The Gold-Rich Eu5Au16(Au/In)6 Structure. **2015**, 54, 8187-96	18
1526	Cation-Poor Complex Metallic Alloys in Ba(Eu)-Au-Al(Ga) Systems: Identifying the Keys that Control Structural Arrangements and Atom Distributions at the Atomic Level. **2015**, 54, 10296-308	23
1525	ACdCO3F (A = K and Rb): new noncentrosymmetric materials with remarkably strong second-harmonic generation (SHG) responses enhanced via □nteraction. **2015**, 5, 84754-84761	53
1524	A first-principles study of Pt thin films on SrTiO3(100): Support effects on CO adsorption. **2015**, 142, 124704	9
1523	Discovery of □MnP4 and the Polymorphism of Manganese Tetraphosphide. **2015**, 54, 8761-8	6
1522	Ab initio study of Ga-GaN system: Transition from adsorbed metal atoms to a metal□emiconductor junction. **2015**, 33, 061101	4
1521	A new form of Ca3P2 with a ring of Dirac nodes. **2015**, 3, 083602	244
1520	Sr14Sn3As12 and Eu14Sn3As12: enantiomorph-like Zintl compounds. **2015**, 54, 8875-7	5
1519	A chemical link between Ge□b□□e and In□b□□e phase-change materials. **2015**, 3, 9519-9523	34
1518	Synthesis, crystal structure, and bonding analysis of the hypoelectronic cubic phase Ca5Pd6Ge6. **2015**, 54, 9098-104	4
1517	Crystal feature and electronic structure of novel mixed alanate LiCa(AlH4)3: a density functional theory investigation. **2015**, 5, 16439-16445	5
1516	Estimation of bonding nature using diamagnetic susceptibility. **2015**, 51, 8691-4	4
1515	Li-Filled, B-Substituted Carbon Clathrates. **2015**, 137, 12639-52	26
1514	Interfacial chemical bonding between carbon nanotube and aluminum substrate modulated by alloying elements. **2015**, 59, 1-6	3

1513	A new representative of the cubic parkerites family: Synthesis, crystal and electronic structure of Pt3Bi2Se2. **2015**, 651, 193-199	5
1512	Parameter determination procedure for extended Hčkel approximation and its application for solid-state electrolytes. **2015**, 21, 169	2
1511	Distorted phosphorus and copper square-planar layers in LaCu1+xP2 and LaCu4P3: synthesis, crystal structure, and physical properties. **2015**, 54, 890-7	25
1510	Putting DFT to the test: a first-principles study of electronic, magnetic, and optical properties of Co3O4. **2015**, 11, 64-72	65
1509	Spin-gapless semiconducting graphitic carbon nitrides: A theoretical design from first principles. **2015**, 84, 1-8	61
1508	Crystal structure and bonding in BaAu5Ga2 and AeAu4+xGa3-x (Ae = Ba and Eu): hexagonal diamond-type Au frameworks and remarkable cation/anion partitioning in the Ae-Au-Ga systems. **2015**, 54, 1010-8	19
1507	Investigation of magnetic properties and electronic structure of layered-structure borides AlT2B2 (T=Fe, Mn, Cr) and AlFe2MnxB2. **2015**, 224, 52-61	75
1506	GeP and (Ge1Sn)(P1Ge) (x0.12, y0.05): Synthesis, structure, and properties of two-dimensional layered tetrel phosphides. **2015**, 224, 62-70	38
1505	Phase transitions, mechanical properties and electronic structures of novel boron phases under high-pressure: a first-principles study. **2014**, 4, 6786	13
1504	Novel metastable compounds in the Zr-B system: an ab initio evolutionary study. **2015**, 17, 1180-8	19
1503	Lithiation-induced zinc clustering of Zn3, Zn12, and Zn18 units in Zintl-like Ca~30Li3+xZn60-x (x = 0.44-1.38). **2015**, 54, 922-9	2
1502	Experimental and theoretical investigations for site preference and anisotropic size change of RE11Ge4In6Mx (RE = La, Ce; M = Li, Ge; x = 1, 1.96). **2015**, 620, 269-276	12
1501	Phase stability of N substituted Li2FeSiO4 electrode material: DFT calculations. **2015**, 96, 290-294	8
1500	Structural modulations in the rare-earth metal digermanides REAl1-xGe2 (RE = Gd-Tm, Lu, Y; 0.8 2015, 54, 722-32	11
1499	Theory of surface chemistry and reactivity of reducible oxides. **2015**, 244, 63-84	49
1498	Homoatomic clustering in T4Ga5 (T = Ta, Nb, Ta/Mo): a story of reluctant intermetallics crystallizing in a new binary structure type. **2015**, 54, 821-31	5
1497	Cationic Site-Preference in the YbCaAlSb (4.81x10.57) Series: Theoretical and Experimental Studies. **2016**, 9,	13
1496	Strain Engineering of the CeNi5 System. **2016**, 2, 39	3

1495	Nitrogen-Rich Manganese Oxynitrides with Enhanced Catalytic Activity in the Oxygen Reduction Reaction. **2016**, 128, 8095-8099	7
1494	Palladium pnictide oxides Nd10Pd3As8O10 and Sm10Pd3As8O10 low temperature structural phase transition and physical properties. **2016**, 4, 6727-6741	0
1493	Electronic and Magnetic Properties of Encapsulated MoS2 Quantum Dots: The Case of Noble Metal Nanoparticle Dopants. **2016**, 17, 1180-94	2
1492	Nanomaterials for Fuel Cell Catalysis. **2016**,	10
1491	Sr2Pd4Al5: Synthesis, Crystal and Electronic Structures, and Chemical Bonding of a Polar Intermetallic Compound. **2016**, 2016, 1108-1114	6
1490	e-TiO, a Novel Stable Polymorph of Titanium Monoxide. **2016**, 128, 1684-1689	2
1489	Band Gap Insensitivity to Large Chemical Pressures in Ternary Bismuth Iodides for Photovoltaic Applications. **2016**, 120, 28924-28932	37
1488	Increased Back-Bonding Explains Step-Edge Reactivity and Particle Size Effect for CO Activation on Ru Nanoparticles. **2016**, 138, 16655-16668	42
1487	Metastable Layered Cobalt Chalcogenides from Topochemical Deintercalation. **2016**, 138, 16432-16442	47
1486	Structural and electronic structures of alkaline-earth transition metal oxynitride perovskites. **2016**, 124, 1056-1062	3
1485	Inherent instability by antibonding coupling in AgSbTe2. **2016**, 55, 041801	9
1484	Caesiumplatinidhydrid, 4 Cs2Pt?CsH: ein intermetallisches Doppelsalz mit Metall-Anionen. **2016**, 128, 15059-15062	
1483	Growth of metalloid aluminum clusters on graphene vacancies. **2016**, 144, 024703	1
1482	Water adsorption on the LaMnO3 surface. **2016**, 144, 064701	4
1481	Comparison of S-adsorption on (111) and (100) facets of Cu nanoclusters. **2016**, 145, 164312	5
1480	Theoretical and experimental investigation of defect formation / migration in Gd2Ti2O7: General rule of oxide-ion migration in A2B2O7 pyrochlore. **2016**, 6, 115003	15
1479	Persistence of polar distortion with electron doping in lone-pair driven ferroelectrics. **2016**, 94,	38
1478	A new type of vanadium carbide V5C3 and its hardening by tuning Fermi energy. **2016**, 6, 21794	16

1477	Electronic hybridisation implications for the damage-tolerance of thin film metallic glasses. **2016**, 6, 36556	21
1476	High-throughput exploration of thermoelectric and mechanical properties of amorphous NbO2 with transition metal additions. **2016**, 120, 045104	9
1475	Several stories from theoretical chemistry with some Russian flavor and implications for theorems of chemistry, vagueness of its concepts, fuzziness of its definitions, iconicity of its language, and peculiarities of its nomenclature. **2016**, 116, 137-160	8
1474	Electronic Structure and Bonding in Co-Based Single and Mixed Valence Oxides: A Quantum Chemical Perspective. **2016**, 55, 3307-15	32
1473	Size Dependence of S-bonding on (111) Facets of Cu Nanoclusters. **2016**, 120, 10268-10274	9
1472	LOBSTER: A tool to extract chemical bonding from plane-wave based DFT. **2016**, 37, 1030-5	1003
1471	Tuning Complexity by Lithiation: A Family of Intergrowth Structures Using Condensed hypho-Icosahedra in the Li-Doped Ca-Zn System. **2016**, 55, 5041-50	3
1470	Electrochemical activity and high ionic conductivity of lithium copper pyroborate Li6CuB4O10. **2016**, 18, 14960-9	11
1469	Understanding and Tuning the Hydrogen Evolution Reaction on Pt-Covered Tungsten Carbide Cathodes. **2016**, 163, F629-F636	13
1468	Electronic and Bonding Properties of LiMn2O4Spinel with Different Surface Orientations and Doping Elements and Their Effects on Manganese Dissolution. **2016**, 163, A1359-A1368	27
1467	Exploring the Real Ground-State Structures of Molybdenum Dinitride. **2016**, 120, 11060-11067	31
1466	Theoretical characterization of the surface composition of ruthenium nanoparticles in equilibrium with syngas. **2016**, 8, 10974-92	34
1465	Peierls-Distorted Ru-Chains and Boron Dumbbells in Nb2RuB2 and Ta2RuB2 from First-Principles Calculations and Experiments. **2016**, 2016, 4104-4110	3
1464	Determining a Structural Distortion and Anion Ordering in La2Si4N6C via Computation and Experiment. **2016**, 55, 9454-60	6
1463	Theoretical and experimental investigation on structural, electronic and magnetic properties of layered MnO. **2016**, 18, 27885-27896	11
1462	The Key Indicator for the Control of Metal Particle Sizes on Supports from First-Principles and Experimental Observation. **2016**, 120, 21879-21887	4
1461	Insight on the oxidation resistance of UO N layers: A density functional study. **2016**, 123, 224-231	10
1460	Li-Ge-H system: Hydrogenation and structural properties of LiGeHx (0. **2016**, 61, 24-31	2

1459	An Icosahedral Quasicrystal and Its 1/0 Crystalline Approximant in the Ca-Au-Al System. **2016**, 55, 10425-104376	
1458	Integrated Studies of Au@Pt and Ru@Pt Core-Shell Nanoparticles by In Situ Electrochemical NMR, ATR-SEIRAS, and SERS. **2016**, 225-251	
1457	Crystal Structure, 7Li NMR, and Structural Relationship of Two Rare-Earth Metal Richer Polar Intermetallics: La15Ge9Li1.50(16) and La7Ge3. **2016**, 37, 1344-1353	1
1456	A2VO(SO4)2 (A = Li, Na) as Electrodes for Li-Ion and Na-Ion Batteries. **2016**, 28, 6637-6643	18
1455	EuAu3Al2: Crystal and Electronic Structures and Spectroscopic, Magnetic, and Magnetocaloric Properties. **2016**, 55, 9057-64	11
1454	Pressure-Stabilized Ir3Ih a Superconducting Potassium Iridide. **2016**, 120, 20033-20039	12
1453	Sulfur to oxygen substitution in BiOCuSe and its effect on the thermoelectric properties. **2016**, 4, 13859-13865	10
1452	Electronic bonding analyses and mechanical strengths of incompressible tetragonal transition metal dinitrides TMN (TM = Ti, Zr, and Hf). **2016**, 6, 36911	17
1451	Stabilization of a Metastable Fibrous Bi21.2(1)(Mn1Cox)20 Phase with Pseudo-Pentagonal Symmetry Prepared Using a Bi Self-Flux. **2016**, 28, 8484-8488	1
1450	Conflict between the Electronic Factors and Structure-Directing Rules in the Intergrowth Structure of Ca4Ag2+xGe4 with x = 1/2. **2016**, 16, 5946-5953	1
1449	An atomic-scale insight into the effects of hydrogen microalloying on the glass-forming ability and ductility of Zr-based bulk metallic glasses. **2016**, 125, 197-205	10
1448	Current-induced phonon renormalization in molecular junctions. **2016**, 94,	8
1447	Experimental and theoretical investigations of the polar intermetallics SrPt3Al2 and Sr2Pd2Al. **2016**, 242, 143-150	12
1446	Experimental and Theoretical Studies on the Crystal Structure of Ternary Copper Arsenides A2Cu3As3 (A = Sr, Eu). **2016**, 2016, 3774-3780	4
1445	Cesium Platinide Hydride 4Cs Pt?CsH: An Intermetallic Double Salt Featuring Metal Anions. **2016**, 55, 14838-14841	11
1444	Structure and Electronic Properties of FeSH Compound under High Pressure. **2016**, 55, 11434-11439	35
1443	Strong Oxygen Participation in the Redox Governing the Structural and Electrochemical Properties of Na-Rich Layered Oxide Na2IrO3. **2016**, 28, 8278-8288	98
1442	Competition between Two High-Density Assemblies of Poly(phenyl)thiols on Au(111). **2016**, 120, 25462-25472	16

1441	Exo-bonded six-membered heterocycle in the crystal structures of RECoGe (RE = La-Nd). **2016**, 45, 18522-18531	3
1440	Extremely Scalable Algorithm for 108-atom Quantum Material Simulation on the Full System of the K Computer. **2016**,	2
1439	Spin-glass behavior of Sn0.9Fe3.1N: An experimental and quantum-theoretical study. **2016**, 6, 055107	11
1438	Formation of Metallic States between Insulating SnO and SnO2. **2016**, 3, 1500334	2
1437	Spin Frustration and Magnetic Ordering from One-Dimensional Stacking of Cr3 Triangles in TiCrIr2B2. **2016**, 55, 5640-8	9
1436	Conjugation-Driven "Reverse Mars-van Krevelen"-Type Radical Mechanism for Low-Temperature C-O Bond Activation. **2016**, 138, 8104-13	62
1435	A DFT+U study on the contribution of 4f electrons to oxygen vacancy formation and migration in Ln-doped CeO2. **2016**, 18, 12938-46	32
1434	Silicon Framework-Based Lithium Silicides at High Pressures. **2016**, 8, 16761-7	11
1433	Transition Metal and Vacancy Defect Complexes in Phosphorene: A Spintronic Perspective. **2016**, 120, 14991-15000	49
1432	Enclathration of [email´protected]4 Tetrahedra in Channels of ZnP Frameworks in La3Zn4P6X (X = Cl, Br). **2016**, 28, 4741-4750	17
1431	The coloring problem in the solid-state metal boride carbide ScB2C2: a theoretical analysis. **2016**, 71, 593-601	4
1430	Significant Lanthanoid Substitution Effect on the Redox Reactivity of the Oxygen-Storage Material BaYMn2O5+ **2016**, 28, 4409-4414	19
1429	Revisiting Ir(CO)3Cl. **2016**, 103, 141-149	8
1428	Possible new metastable Mo2Ga2C and its phase transition under pressure: a density functional prediction. **2016**, 51, 8452-8460	7
1427	How molecular is the chemisorptive bond?. **2016**, 18, 20868-94	34
1426	Defect Tolerance to Intolerance in the Vacancy-Ordered Double Perovskite Semiconductors Cs2SnI6 and Cs2TeI6. **2016**, 138, 8453-64	264
1425	Cu Insertion Into the Mo12 Cluster Compound Cs2Mo12Se14: Synthesis, Crystal and Electronic Structures, and Physical Properties. **2016**, 55, 6616-24	14
1424	e-TiO, a Novel Stable Polymorph of Titanium Monoxide. **2016**, 55, 1652-7	35

1423	Nitrogen-Rich Manganese Oxynitrides with Enhanced Catalytic Activity in the Oxygen Reduction Reaction. **2016**, 55, 7963-7	42
1422	Relativistic electronic structure and band alignment of BiSI and BiSeI: candidate photovoltaic materials. **2016**, 4, 2060-2068	97
1421	New ternary tantalum borides containing boron dumbbells: Experimental and theoretical studies of Ta2OsB2 and TaRuB. **2016**, 242, 28-33	7
1420	The role of terminations and coordination atoms on the pseudocapacitance of titanium carbonitride monolayers. **2016**, 18, 4376-84	23
1419	Crystal Chemistry of the New Families of Interstitial Compounds R6Mg23C (R = La, Ce, Pr, Nd, Sm, or Gd) and Ce6Mg23Z (Z = C, Si, Ge, Sn, Pb, P, As, or Sb). **2016**, 55, 191-204	5
1418	A combined computational and experimental investigation of Mg doped □-Fe2O3. **2016**, 18, 781-91	13
1417	Two theorems about C2 and some more. **2016**, 114, 1423-1444	9
1416	Two New Non-centrosymmetric n = 3 Layered Dion□acobson Perovskites: Polar RbBi2Ti2NbO10 and Nonpolar CsBi2Ti2TaO10. **2016**, 28, 2424-2432	38
1415	Mixed Valence Tin Oxides as Novel van der Waals Materials: Theoretical Predictions and Potential Applications. **2016**, 6, 1501190	66
1414	Structure and Bonding of an Intergrowth Phase Ca7Ag2+xGe7□ (x □2/3) Featuring a Zintl-Type Polyanionic Chain. **2016**, 2016, 169-176	4
1413	2D 31P solid state NMR spectroscopy, electronic structure and thermochemistry of PbP7. **2016**, 235, 139-144	2
1412	Molecular structure and vibrations of NTCDA monolayers on Ag(111) from density-functional theory and infrared absorption spectroscopy. **2016**, 18, 6316-28	23
1411	Influence of alloying elements on the stability and dehydrogenation properties on Y(BH4)3 by first principles calculations. **2016**, 41, 1662-1671	2
1410	Role of 5f electrons in the structural stability of light actinide (Th-U) mononitrides under pressure. **2016**, 18, 8682-91	7
1409	Nickel cluster functionalised carbon nanotube for CO molecule detection: a theoretical study. **2016**, 114, 671-680	7
1408	Gold as a 6p-Element in Dense Lithium Aurides. **2016**, 138, 4046-52	70
1407	High-Pressure Synthesis and Characterization of Incompressible Titanium Pernitride. **2016**, 28, 1616-1620	61
1406	New insight into the intrinsic instability of fcc ZrH2 by energy-resolved local bonding analysis. **2016**, 6, 19150-19154	4

1405	Atomic level understanding of site-specific interactions in Polyaniline/TiO2 composite. **2016**, 645, 144-149	6
1404	Homogeneity ranges and physical properties of ternary Laves phases R x Zr 1-x Ni 2 (R ´=´Gd□u). **2016**, 661, 490-494	2
1403	First-principles investigation of the magnetic structures and pressure-induced magnetic phase transition in magnetocaloric MnRhAs. **2016**, 112, 34-38	0
1402	The development of two dimensional group IV chalcogenides, blocks for van der Waals heterostructures. **2016**, 8, 1169-78	49
1401	New insights into the application of the valence rules in Zintl phases□Crystal and electronic structures of Ba7Ga4P9, Ba7Ga4As9, Ba7Al4Sb9, Ba6CaAl4Sb9, and Ba6CaGa4Sb9. **2016**, 236, 116-122	7
1400	The intriguing question of anionic redox in high-energy density cathodes for Li-ion batteries. **2016**, 9, 984-991	346
1399	Atomic interactions in the intermetallic catalyst GaPd. **2016**, 114, 1250-1259	20
1398	Ce11Ge3.73(2)In6.27: Solid-state synthesis, crystal structure and site-preference. **2016**, 236, 195-202	10
1397	Influence of Thermally Activated Solid-State Crystal-to-Crystal Structural Transformation on the Thermoelectric Properties of the Ca5□YbxAl2Sb6 (1.0≤x≤5.0) System. **2017**, 29, 1384-1395	13
1396	Local Bi ordering in MOVPE grown Ga(As,Bi) investigated by high resolution scanning transmission electron microscopy. **2017**, 6, 22-28	15
1395	Magnetocaloric Behavior in Ternary Europium Indides EuT5In: Probing the Design Capability of First-Principles-Based Methods on the Multifaceted Magnetic Materials. **2017**, 29, 2599-2614	20
1394	EuNi5InH1.5□ (x = 0□1.5): hydrogen induced structural and magnetic transitions. **2017**, 5, 2994-3006	8
1393	Tetrel Bonds in Infinite Molecular Chains by Electronic Structure Theory and Their Role for Crystal Stabilization. **2017**, 121, 1381-1387	13
1392	First-Order Phase Transition in BaNiGe and the Influence of the Valence Electron Count on Distortion of the ThCrSi Structure Type. **2017**, 56, 1173-1185	5
1391	Strengthening materials by changing the number of valence electrons. **2017**, 129, 252-258	6
1390	Establishment of half-metallicity, ferrimagnetic ordering and double exchange interactions in Ni-doped BiFeO3 □A first-principles study. **2017**, 130, 84-90	11
1389	The synthesis of unconventional stoichiometric compounds in the K-Br system at high pressures. **2017**, 19, 7996-8007	13
1388	First-principles calculations on slip system activation in the rock salt structure: electronic origin of ductility in silver chloride. **2017**, 97, 1281-1310	11

1387	Pressure-stabilized hafnium nitrides and their properties. **2017**, 95,	53
1386	Prediction and characterization of the marcasite phase of iron pernitride under high pressure. **2017**, 702, 132-137	19
1385	A stable compound of helium and sodium at high pressure. **2017**, 9, 440-445	199
1384	Electronic Structure and Comparative Properties of LiNixMnyCozO2 Cathode Materials. **2017**, 121, 6002-6010	89
1383	Understanding surface site structures and properties by first principles calculations: an experimental point of view!. **2017**, 53, 4296-4303	14
1382	Unerwartete Ge-Ge-Kontakte in der zweidimensionalen Phase Ge4Se3Te und Analyse ihres chemischen Ursprungs mittels Energiedichte(DOE)-Funktion. **2017**, 129, 10338-10342	1
1381	Basic Quantum-Chemical Concepts, The Chemical Bond Revisited (Jointly Written with I. Tranca). **2017**, 173-207	1
1380	Unexpected Ge-Ge Contacts in the Two-Dimensional Ge Se Te Phase and Analysis of Their Chemical Cause with the Density of Energy (DOE) Function. **2017**, 56, 10204-10208	45
1379	Synergic effects of VLi and Ti doping on hydrogen desorption on LiBH4 (010) surface: A first-principles investigation. **2017**, 42, 18442-18451	3
1378	111-Type Semiconductor ReGaSi Follows 14e Rules. **2017**, 56, 5165-5172	7
1377	Group-IV (Si, Ge, and Sn)-doped AgAlTe2for intermediate band solar cell from first-principles study. **2017**, 32, 065007	11
1376	How silver segregation stabilizes 1D surface gold oxide: a cluster expansion study combined with ab initio MD simulations. **2017**, 19, 14845-14853	17
1375	Plane-Wave Density Functional Theory Meets Molecular Crystals: Thermal Ellipsoids and Intermolecular Interactions. **2017**, 50, 1231-1239	41
1374	Fast Prediction of CO Binding Energy via the Local Structure Effect on PtCu Alloy Surfaces. **2017**, 33, 8700-8706	20
1373	Phase-dependent radiation-resistant behavior of BaTiO3: An in´situ X-ray diffraction study. **2017**, 100, 4263-4269	6
1372	Requirements for reversible extra-capacity in Li-rich layered oxides for Li-ion batteries. **2017**, 10, 266-274	192
1371	Syntheses, structures, and properties of sulfides constructed by SbS4 teeter-totter polyhedra: Ba3La4Ga2Sb2S15 and BaLa3GaSb2S10. **2017**, 4, 123-130	10
1370	High-Pressure NiAs-Type Modification of FeN. **2017**, 56, 7302-7306	36

1369	Bonding analyses of unconventional carbon allotropes. **2017**, 121, 154-162	18
1368	Potential high- superconducting lanthanum and yttrium hydrides at high pressure. **2017**, 114, 6990-6995	387
1367	Polar Intermetallics Pr Co Ge and Pr Co Ge with Planar Hydrocarbon-Like Metal Clusters. **2017**, 23, 10516-10521	4
1366	Phase stability and electronic structure of UMo2Al20: A first-principles study. **2017**, 493, 147-153	9
1365	Superconductivity Induced by Oxygen Doping in Y2O2Bi. **2017**, 129, 10257-10260	
1364	Difficulty of long-standing n-type conductivity in equilibrium and non-equilibrium CuCl: A first-principles study. **2017**, 381, 2743-2747	3
1363	Crystal Structures of CaBN at High Pressures. **2017**, 56, 7449-7453	1
1362	Zweidimensionales Haeckelit-NbS2 ein diamagnetischer Halbleiter mit Nb4+-Ionen und hoher Ladungsträgermobilität. **2017**, 129, 10348-10352	
1361	Local Bonding Influence on the Band Edge and Band Gap Formation in Quaternary Chalcopyrites. **2017**, 4, 1700080	24
1360	Ultra-stiff metallic glasses through bond energy density design. **2017**, 29, 265502	9
1359	Effect of MultiSubstitution on the Thermoelectric Performance of the CaYbSbGe (0≤x≤0.9; 0≤y≤0.3; 0≤z≤3) System: Experimental and Theoretical Studies. **2017**, 56, 7099-7110	12
1358	Two-Dimensional Haeckelite NbS : A Diamagnetic High-Mobility Semiconductor with Nb Ions. **2017**, 56, 10214-10218	24
1357	CO Adsorption on (110)-(1 2) Missing-Row Reconstructed Surfaces of Pd, Au, and Pd3Au: Electronic Structures and Vibrational Frequencies. **2017**, 86, 044712	2
1356	Superconductivity Induced by Oxygen Doping in Y O Bi. **2017**, 56, 10123-10126	7
1355	Amorphous phase stability and the interplay between electronic structure and topology. **2017**, 131, 131-140	12
1354	Cationic order versus La-O covalency in LaA(Ca,Ba)VMoO6 double perovskites. **2017**, 95,	5
1353	In Operando Self-Healing of Perovskite Electrocatalysts: A Case Study of SrCoO3 for the Oxygen Evolution Reaction. **2017**, 34, 1600280	9
1352	Quantum mechanically guided design of amorphous SiAlM (M = 3d metals) anodes for Li ion batteries. **2017**, 303, 47-51	5

1351	Theoretical insights into the interaction between RuPt (n=4, 7 and 9) clusters and [BMIM] based ionic liquids: Effect of anion. **2017**, 74, 117-124	2
1350	Crystal structure, homogeneity range and electronic structure of rhombohedral Mn5Al8. **2017**, 232, 601-610	7
1349	Structural design principles for low hole effective mass s-orbital-based p-type oxides. **2017**, 5, 5772-5779	46
1348	Synthesis and structural characterization of the Zintl phases Na3Ca3TrPn4, Na3Sr3TrPn4, and Na3Eu3TrPn4 (Tr=Al, Ga, In; Pn=P, As, Sb). **2017**, 249, 160-168	6
1347	Determination of Crystal Structure of Graphitic Carbon Nitride: Ab Initio Evolutionary Search and Experimental Validation. **2017**, 29, 2694-2707	51
1346	High-Throughput Survey of Ordering Configurations in MXene Alloys Across Compositions and Temperatures. **2017**, 11, 4407-4418	97
1345	AlMB (M = Cr, Mn, Fe, Co, Ni): a group of nanolaminated materials. **2017**, 29, 155402	44
1344	Phase diagram, stability and electronic properties of an FeB system under high pressure: a first principles study. **2017**, 7, 15986-15991	18
1343	Enhancement of the Thermoelectric Properties of FeGa-type Structures with Group 6 Transition Metals: A Computational Exploration. **2017**, 56, 4229-4237	4
1342	Anisotropic Electronic Structure and Transport Properties of the H-0 Hyperhoneycomb Lattice. **2017**, 121, 1928-1933	1
1341	Quasimolecules in Compressed Lithium. **2017**, 129, 992-995	15
1340	Computational Design of Rare-Earth-Free Magnets with the Ti3Co5B2-Type Structure. **2017**, 29, 2535-2541	18
1339	Synthesis, Crystal Structure, and Properties of LaZnP and LaMgZnP. **2017**, 56, 783-790	17
1338	Electrochemical Energy Generation and Storage as Seen by In-Situ NMR. **2017**, 331-363	2
1337	Layered Structures and Disordered Polyanionic Nets in the Cation-Poor Polar Intermetallics CsAu1.4Ga2.8 and CsAu2Ga2.6. **2017**, 17, 693-700	4
1336	Stability and electronic properties of two-dimensional indium iodide. **2017**, 95,	7
1335	A Chemical Understanding of the Band Convergence in Thermoelectric CoSb3 Skutterudites: Influence of Electron Population, Local Thermal Expansion, and Bonding Interactions. **2017**, 29, 1156-1164	38
1334	Activation of surface oxygen sites on an iridium-based model catalyst for the oxygen evolution reaction. **2017**, 2,	274

1333	Quasimolecules in Compressed Lithium. **2017**, 56, 972-975	25
1332	Crystal structure, electronic structure and physical properties of the new quaternary chalcogenides Tl2NdAg3Se4 and Tl2NdAg3Te4. **2017**, 4, 315-323	6
1331	Prediction of superconducting iron-bismuth intermetallic compounds at high pressure. **2017**, 8, 2226-2234	20
1330	Structural, electronic and optical properties of famatinite and enargite Cu3SbS4 under pressure: A theoretical investigation. **2017**, 254, 1600608	3
1329	Quantification of cation-anion interactions in crystalline monopotassium and monosodium glutamate salts. **2017**, 19, 28647-28652	4
1328	Scaling Relations for Acidity and Reactivity of Zeolites. **2017**, 121, 23520-23530	56
1327	First-Principles Chemical Bonding Study of Manganese Carbodiimide, MnNCN, As Compared to Manganese Oxide, MnO. **2017**, 121, 7778-7786	15
1326	Ether auf Si(001): Ein Paradebeispiel fî.die Gemeinsamkeiten zwischen Oberflîchenwissenschaften und organischer Molekîchemie. **2017**, 129, 15347-15351	3
1325	Metastable Stacking-Polymorphism in GeSbTe. **2017**, 56, 11990-11997	13
1324	First-principles investigation of competing magnetic interactions in (Mn,Fe)Ru2Sn Heusler solid solutions. **2017**, 96,	4
1323	Basic Properties of Well-Known Intermetallics and Some New Complex Magnetic Intermetallics. **2017**, 345-403	1
1322	Ultrafast charge transfer dynamics pathways in two-dimensional MoS-graphene heterostructures: a core-hole clock approach. **2017**, 19, 29954-29962	23
1321	On atomic mechanisms governing the oxidation of BiTe. **2017**, 29, 485705	22
1320	Single and double-doping effects on the thermoelectric properties of two Zintl compounds: EuBiSn and EuKBiSn. **2017**, 46, 11840-11850	8
1319	Revisiting the Si-Te System: SiTe Finally Found by Means of Experimental and Quantum-Chemical Techniques. **2017**, 56, 11398-11405	14
1318	A curved pathway for oxygen interstitial diffusion in aluminum. **2017**, 140, 47-54	8
1317	Phase Stability, Phase Mixing, and Phase Separation in Fluorinated Alkaline Earth Hydrides. **2017**, 121, 21806-21820	6
1316	Density Functional Theory. **2017**, 1-28	

1315	Chemical Bonding in Solids. **2017**, 405-489	2
1314	Tailoring the Electronic Band Gap and Band Edge Positions in the C2N Monolayer by P and As Substitution for Photocatalytic Water Splitting. **2017**, 121, 22216-22224	49
1313	Ethers on Si(001): A Prime Example for the Common Ground between Surface Science and Molecular Organic Chemistry. **2017**, 56, 15150-15154	22
1312	Theoretical study of stability and superconductivity of ScHn (n=4□8) at high pressure. **2017**, 96,	31
1311	Noble gas bond and the behaviour of XeO under pressure. **2017**, 19, 27463-27467	11
1310	Origin of Structural Degradation During Cycling and Low Thermal Stability of Ni-Rich Layered Transition Metal-Based Electrode Materials. **2017**, 121, 22628-22636	123
1309	Ab initio study of the likely orientation relationships of interphase and homophase interfaces in a two-phase HCP + BCC Mg-Li alloy. **2017**, 139, 406-411	9
1308	First-Principles Study of Chemical Mixtures of CaCl and MgCl Hydrates for Optimized Seasonal Heat Storage. **2017**, 121, 20576-20590	15
1307	First-principle study of pressure-induced phase transitions and electronic properties of electride Y2C. **2017**, 266, 34-38	5
1306	Efficient PAW-based bond strength analysis for understanding the In/Si(111)(8 □2) - (4 □1) phase transition. **2017**, 38, 2276-2282	9
1305	Two-Dimensional Hexagonal Sheet of TiO2. **2017**, 29, 8594-8603	51
1304	Theoretical investigation of phase separation in thermoelectric AgSbTe2. **2017**, 56, 081201	1
1303	Chemical Aspects of Itinerant Magnetism. **2017**, 1-9	1
1302	Equiatomic indides REIrIn (RE=La, Pr, Nd, Er□Yb) □Crystal and electronic structure. **2017**, 72, 631-638	4
1301	Revealing the Nature of Bonding in Rare-Earth Transition-Metal Tellurides by Means of Methods Based on First Principles. **2017**, 2017, 3395-3400	13
1300	First-principles study on adsorption structure and electronic state of stanene on □-alumina surface. **2017**, 56, 095701	6
1299	Chemical Origin of Termination-Functionalized MXenes: Ti3C2T2 as a Case Study. **2017**, 121, 19254-19261	118
1298	Single-Layer TlO: A Metal-Shrouded 2D Semiconductor with High Electronic Mobility. **2017**, 139, 11694-11697	60

1297	The Influence of the Valence Electron Concentration on the Structural Variation of the Laves Phases MgNi2−xGex. **2017**, 643, 1424-1430	8
1296	Diffusion of a Single Platinum Atom on Light-Element-Doped Graphene. **2017**, 121, 17787-17795	13
1295	A Polyselenide with a Novel Se78− Unit: the Structure of Sr19−xPbxGe11Se44 with x = 5.0 and 6.4. **2017**, 2017, 5515-5520	3
1294	Investigation into Structural Phase Transitions in Layered Titanium-Oxypnictides by a Computational Phonon Analysis. **2017**, 56, 13732-13740	4
1293	Thermoelectric properties and thermal stability of layered chalcogenides, TlScQ, Q = Se, Te. **2017**, 46, 17053-17060	7
1292	Reducing the stochasticity of crystal nucleation to enable subnanosecond memory writing. **2017**, 358, 1423-1427	338
1291	Bimetallic Effect of Single Nanocatalysts Visualized by Super-Resolution Catalysis Imaging. **2017**, 3, 1189-1197	47
1290	Packing of Russian doll clusters to form a nanometer-scale CsCl-type compound in a Cr−nSn complex metallic alloy. **2017**, 5, 7215-7221	4
1289	First-principles description of van der Waals bonded spin-polarized systems using the vdW-DF+U method: Application to solid oxygen at low pressure. **2017**, 95,	5
1288	Crystal structure of and displacive phase transition in tungsten nitride WN. **2017**, 722, 517-524	8
1287	Constrained-Orbital Density Functional Theory. Computational Method and Applications to Surface Chemical Processes. **2017**, 13, 3561-3574	14
1286	Ultrastrong Boron Frameworks in ZrB : A Highway for Electron Conducting. **2017**, 29, 1604003	50
1285	Adsorption of transition metal adatoms on h-BN/Rh(111): Implications for nanocluster self-assembly. **2017**, 280, 220-231	11
1284	Insight into chemoselectivity of nitroarene hydrogenation: A DFT-D3 study of nitroarene adsorption on metal surfaces under the realistic reaction conditions. **2017**, 392, 456-471	14
1283	Shape, electronic structure and steric effects of organometallic nanocatalysts: relevant tools to improve the synergy between theory and experiment. **2017**, 46, 378-395	14
1282	First-principles phase diagram calculations for the rocksalt-structure quasibinary systems TiN-ZrN, TiN-HfN and ZrN-HfN. **2017**, 29, 035401	28
1281	Magnetic control of single transition metal doped MoS2 through H/F chemical decoration. **2017**, 422, 243-248	5
1280	Alloy Systems and Compounds Containing Rare Earth Metals and Carbon. **2017**, 1-263	7

1279	Decentral distribution of helium in □SiC: Studied by density functional theory. **2017**, 13, 35-41	3
1278	Single-bonded allotrope of nitrogen predicted at high pressure. **2017**, 96,	27
1277	Low-temperature synthesis and rational design of nitrides and oxynitrides for novel functional material development. **2017**, 125, 552-558	11
1276	A Review on Disorder-Driven Metal-Insulator Transition in Crystalline Vacancy-Rich GeSbTe Phase-Change Materials. **2017**, 10,	38
1275	The Pressing Role of Theory in Studies of Compressed Matter. **2017**, 571-605	6
1274	Intermetallic Compounds and Alloy Bonding Theory Derived from Quantum Mechanical One-Electron Models. **2017**, 1-72	
1273	Mechanistic Quantification of Thermodynamic Stability and Mechanical Strength for Two-Dimensional Transition-Metal Carbides. **2018**, 122, 4710-4722	22
1272	CsMnAs: A Layered Tetragonal Transition-Metal Pnictide Compound with an Antiferromagnetic Ground State. **2018**, 57, 3206-3214	3
1271	2D Chiroptical Nanostructures for High-Performance Photooxidants. **2018**, 28, 1707237	26
1270	Electronic Origin and Kinetic Feasibility of the Lattice Oxygen Participation During the Oxygen Evolution Reaction on Perovskites. **2018**, 9, 1473-1479	46
1269	Effects of alloying elements on the stability and mechanical properties of Fe3Al from first-principles calculations. **2018**, 146, 303-309	7
1268	The Large Second-Harmonic Generation of LiCs PO is caused by the Metal-Cation-Centered Groups. **2018**, 57, 3933-3937	40
1267	Insights into exfoliation possibility of MAX phases to MXenes. **2018**, 20, 8579-8592	108
1266	Anisotropic lattice softening near the structural phase transition in the thermosalient crystal 1,2,4,5-tetrabromobenzene. **2018**, 20, 8523-8532	23
1265	Ternary Bismuthide SrPtBi2: Computation and Experiment in Synergism to Explore Solid-State Materials. **2018**, 122, 5057-5063	2
1264	High Pressure and High Temperature Synthesis of the Iron Pernitride FeN. **2018**, 57, 6245-6251	36
1263	Intricate Li-Sn Disorder in Rare-Earth Metal-Lithium Stannides. Crystal Chemistry of RELiSn (RE = La-Nd, Sm; x 2018, 57, 5632-5641	2
1262	Phonon-mediated stabilization and softening of 2D transition metal carbides: case studies of TiCO and MoCO. **2018**, 20, 14608-14618	6

1261	Crystal Chemistry and Photocatalytic Properties of RESTe (RE = Gd, Ho, Er, Tm): Experimental and Theoretical Investigations. **2018**, 57, 5343-5351	10
1260	HT-NbOsB: Experimental and Theoretical Investigations of a Boride Structure Type Containing Boron Chains and Isolated Boron Atoms. **2018**, 2018, 3297-3303	1
1259	Room-temperature ductile inorganic semiconductor. **2018**, 17, 421-426	147
1258	DFT study of new biologically important oxidovanadium (IV) complexes of nitro-substituted benzohydroxamate ligands. **2018**, 18, 149-163	0
1257	Revisiting building block ordering of long-period stacking ordered structures in Mg□Al alloys. **2018**, 152, 96-106	14
1256	The Large Second-Harmonic Generation of LiCs2PO4 is caused by the Metal-Cation-Centered Groups. **2018**, 130, 3997-4001	15
1255	Experimental and Theoretical Studies of the Metallic Conductivity in Cubic PbVO3 under High Pressure. **2018**, 87, 024801	18
1254	Electronic structure, defect formation energy, and photovoltaic properties of wurtzite-derived CuGaO2. **2018**, 123, 161584	10
1253	First principles study on elastic and electronic properties of bialkali alanates M2M?AlH6. **2018**, 43, 3862-3870	8
1252	Zintl Ions within Framework Channels: The Complex Structure and Low-Temperature Transport Properties of NaGe. **2018**, 57, 2002-2012	7
1251	Structural, electronic, vibration and elastic properties of the layered AgInPS semiconducting crystal - DFT approach.. **2018**, 8, 6965-6977	10
1250	Meta-screening and permanence of polar distortion in metallized ferroelectrics. **2018**, 97,	24
1249	Crystal Structures and Electronic Properties of Xe□l Compounds at High Pressure. **2018**, 122, 2941-2950	4
1248	Engineering the Kondo state in two-dimensional semiconducting phosphorene. **2018**, 97,	3
1247	First-principles study of Cs/Rb co-doped FAPbI3 stability and degradation in the presence of water and oxygen. **2018**, 5, 026203	3
1246	Pt-Bi Antibonding Interaction: The Key Factor for Superconductivity in Monoclinic BaPtBi. **2018**, 57, 1698-1701	4
1245	The Mineral St□zite: a Zintl-Phase or Polar Intermetallic? A Case Study Using Experimental and Quantum-Chemical Techniques. **2018**, 57, 412-421	10
1244	Ternary Iodido Bismuthates and the Special Role of Copper. **2018**, 57, 633-640	23

1243	Structure Transformation and Cerium-Substituted Optical Response across the Carbonitridosilicate Solid Solution (LaY)SiNC (□ = 0-0.5). **2018**, 57, 519-527	1
1242	Effect of boron on the hydrogen-induced grain boundary embrittlement in □-Fe. **2018**, 43, 1909-1925	10
1241	Interplay of Structural and Bonding Characters in Thermal Conductivity and Born-Effective Charge of Transition Metal Dichalcogenides. **2018**, 122, 2521-2527	7
1240	Covalency and spin-orbit coupling driven magnetism in the double-perovskite iridates Sr2MIrO6 (M=Ca, Mg). **2018**, 97,	8
1239	The structural, electronic, magnetic and optical properties of the new promising spintronic material Bi0.92Tb0.08FeO3: A first-principles approach. **2018**, 145, 244-251	4
1238	Electron donation mechanism of superior Cs-supported oxides for catalytic soot combustion. **2018**, 337, 654-660	26
1237	Correlating Itinerant Magnetism in RCoPn Pnictides (R = La, Ce, Pr, Nd, Eu, Ca; Pn = P, As) to Their Crystal and Electronic Structures. **2018**, 51, 230-239	9
1236	Large thermoelectric power factor from crystal symmetry-protected non-bonding orbital in half-Heuslers. **2018**, 9, 1721	77
1235	Investigation of the GaN/Al2O3 Interface by First Principles Calculations. **2018**, 255, 1700323	5
1234	Magnetic ordering and metal-atom site preference in tetragonal CrMnAs: Electronic correlation effects. **2018**, 39, 1585-1593	
1233	Two-Dimensional Be2C with Octacoordinate Carbons and Negative Poisson□ Ratio. **2018**, 122, 7959-7967	14
1232	CO Adsorption Site Preference on Platinum: Charge Is the Essence. **2018**, 8, 3770-3774	31
1231	Unconventional two-dimensional germanium dichalcogenides. **2018**, 10, 7363-7368	21
1230	AAuAl (A = Ca, Sc, and Ti): Peierls Distortion, Atomic Coloring, and Structural Competition. **2018**, 57, 4039-4049	0
1229	Two-dimensional ferroelectricity and switchable spin-textures in ultra-thin elemental Te multilayers. **2018**, 5, 521-528	68
1228	First-principles insights into tin-based two-dimensional hybrid halide perovskites for photovoltaics. **2018**, 6, 5652-5660	50
1227	A novel dual phase membrane 40 wt% Nd0.6Sr0.4CoO3□60 wt% Ce0.9Nd0.1O2□ design, synthesis and properties. **2018**, 6, 84-92	24
1226	Pressure-Induced Polymerization of CO in Lithium-Carbon Dioxide Phases. **2018**, 140, 413-422	9

1225	Ab initio modeling of MAX phase solid solutions using the special quasirandom structure approach. **2018**, 20, 1173-1180	10
1224	Chemical Pressure Maps of Molecules and Materials: Merging the Visual and Physical in Bonding Analysis. **2018**, 14, 104-114	14
1223	Potential Semiconducting and Superconducting Metastable Si3C Structures under Pressure. **2018**, 30, 421-427	4
1222	Competing ferromagnetic and anti-ferromagnetic interactions in iron nitride Fe2N. **2018**, 449, 582-589	3
1221	Theoretical insights into acetylene adsorption on nanoporous gold surfaces: Role of residual silver. **2018**, 434, 735-743	
1220	First-Principles Study of BCC/FCC Phase Transition Promoted by Interstitial Carbon in Iron. **2018**, 59, 870-875	11
1219	Effect of Impurities on the Formation Energy of Point Defects in the TiAl Alloy. **2018**, 127, 1046-1058	8
1218	Synthesis, Crystal Structure, and Chemical-Bonding Analysis of BaZn(NCN)2. **2018**, 6, 1	19
1217	A unique metallic phase of HS at high-pressure: sulfur in three different local environments. **2018**, 20, 26344-26350	6
1216	A synergetic stabilization and strengthening strategy for two-dimensional ordered hybrid transition metal carbides. **2018**, 20, 29684-29692	7
1215	A predictive modeling study of the impact of chemical doping on the strength of a Ag/ZnO interface. **2018**, 124, 235304	
1214	Dynamical stabilization in delafossite nitrides for solar energy conversion. **2018**, 6, 20852-20860	13
1213	Structure stabilization effect of configuration entropy in cubic WN. **2018**, 20, 29243-29248	1
1212	Insight into the intercalation mechanism of WSe2 onions toward metal ion capacitors: sodium rivals lithium. **2018**, 6, 21605-21617	27
1211	Optimizing special quasirandom structure (SQS) models for accurate functional property prediction in disordered 2D alloys. **2018**, 30, 485402	1
1210	High-Pressure Behavior of Lead Cyanamide PbNCN. **2018**, 644, 1881-1885	2
1209	An Ab Initio Study of Connections between Tensorial Elastic Properties and Chemical Bonds in (210) Grain Boundaries in NiSi. **2018**, 11,	3
1208	High-throughput first-principles-calculations based estimation of lithium ion storage in monolayer rhenium disulfide. **2018**, 1,	15

1207	Magnetic origin of phase stability in cubic MoN. **2018**, 113, 221901	6
1206	Beyond the molecular movie: Dynamics of bands and bonds during a photoinduced phase transition. **2018**, 362, 821-825	50
1205	General rules of the sub-band gaps in group-IV (Si, Ge, and Sn)-doped I-III-VI2-type chalcopyrite compounds for intermediate band solar cell: A first-principles study. **2018**, 236-237, 147-152	12
1204	Cage-like $text{N}_{10}^{6-}$ salt with N-N single bonds. **2018**, 124, 67004	2
1203	Interplay between Phonons and Anisotropic Elasticity Drives Negative Thermal Expansion in PbTiO_{3}. **2018**, 121, 255901	13
1202	Revealing Tendencies in the Electronic Structures of Polar Intermetallic Compounds. **2018**, 8, 80	18
1201	Interfacial Interaction between Carbon Nanotube and Stoichio- and Nonstoichiometric Ceramic Surfaces by Ab-Initio Calculations. **2018**, 59, 1684-1690	1
1200	Ab Initio Prediction of Atomic Location of Third Elements in B2-Type TiNi. **2018**, 59, 353-358	1
1199	Enhancing the Thermoelectric Properties of Layered Bi2O2Q (Q = S, Se): the Effect of Mixed Chalcogen Net. **2018**, 73, 1684-1689	2
1198	Origin of the structural phase transition in single-crystal TaTe2. **2018**, 98,	11
1197	Chemical Bonding of Crystalline LnB (Ln = La-Lu) and Its Relationship with LnB Gas-Phase Complexes. **2018**, 57, 12999-13008	39
1196	High-Throughput Screening of Magnetic Antiperovskites. **2018**, 30, 6983-6991	19
1195	On Fe-Fe Dumbbells in the Ideal and Real Structures of FeGa. **2018**, 57, 12908-12919	23
1194	Not Just Par for the Course: 73 Quaternary Germanides RE M XGe (RE = La-Nd, Sm, Gd-Tm, Lu; M = Mn-Ni; X = Ag, Cd) and the Search for Intermetallics with Low Thermal Conductivity. **2018**, 57, 14249-14259	9
1193	Magnetic Moments and Electron Transport through Chromium-Based Antiferromagnetic Nanojunctions. **2018**, 11,	2
1192	Synthesis, Crystal Structure, and Liquid Exfoliation of Layered Lanthanide Sulfides KLnCuS (Ln = La, Ce, Pr, Nd, Sm). **2018**, 57, 13594-13605	2
1191	A novel class of oxynitrides stabilized by nitrogen dimer formation. **2018**, 8, 14471	1
1190	Bonding Hierarchy Gives Rise to High Thermoelectric Performance in Layered Zintl Compound BaAu2P4. **2018**, 30, 7760-7768	21

1189	Study of the Chemical Bond in Li2 yFe1 xMnxSiO4 (x = 0.0, 0.5, 1.0; y = 0.0, 2.0) by the Method of Computer Simulation. **2018**, 44, 455-463	1
1188	Structural-Distortion-Driven Magnetic Transformation from Ferro- to Ferrimagnetic Iron Chains in B6-based Nb6FeIr6B8. **2018**, 130, 10480-10484	0
1187	New Bonding Model of Radical Adsorbate on Lattice Oxygen of Perovskites. **2018**, 9, 6321-6325	21
1186	Thermodynamical Stability of Plutonium Monoxide with Carbon Substitution. **2018**, 122, 22821-22828	6
1185	An Obscured or Nonexistent Binary Intermetallic, Co7Pr17, Its Existent Neighbor Co2Pr5, and Two New Ternaries in the System Co/Sn/Pr, CoSn3Pr1 , and Co2 Sn7Pr3. **2018**, 18, 6273-6283	2
1184	Tin(ii) oxide carbodiimide and its relationship to SnO. **2018**, 47, 13378-13383	11
1183	Simple Route to Metal cyclo-N5 Salt: High-Pressure Synthesis of CuN5. **2018**, 122, 22339-22344	22
1182	Ultrathin MXene Nanosheets Decorated with TiO Quantum Dots as an Efficient Sulfur Host toward Fast and Stable Li-S Batteries. **2018**, 14, e1802443	89
1181	Mixed-valence Compounds: AuO and AuS. **2018**, 19, 2989-2994	5
1180	Polyoxomolybdate-derived carbon-encapsulated multicomponent electrocatalysts for synergistically boosting hydrogen evolution. **2018**, 6, 17874-17881	23
1179	Mg?Si?As: An Unexplored System with Promising Nonlinear Optical Properties. **2018**, 28, 1801589	29
1178	Barium in High Oxidation States in Pressure-Stabilized Barium Fluorides. **2018**, 122, 12448-12453	15
1177	Gd(Co 1-x Ga x) 2 : Synthesis, crystal structures, and investigation of structural transformations and magnetic properties. **2018**, 264, 68-76	3
1176	The Structure and Properties of Magnesium-Phosphorus Compounds Under Pressure. **2018**, 24, 11402-11406	5
1175	Similarity Between Amorphous and Crystalline Phases: The Case of TiO. **2018**, 9, 2985-2990	49
1174	Adsorption and Activation of Methane on the (110) Surface of Rutile-type Metal Dioxides. **2018**, 122, 15359-15381	57
1173	Interplay of covalency, spin-orbit coupling, and geometric frustration in the d3.5 system Ba3LiIr2O9. **2018**, 97,	6
1172	Insights into the Improved High-Voltage Performance of Li-Incorporated Layered Oxide Cathodes for Sodium-Ion Batteries. **2018**, 4, 2124-2139	76

1171	Exotic high-pressure behavior of double nitride CuPN2. **2018**, 152, 217-222	
1170	Pd2Se3 Monolayer: A Promising Two-Dimensional Thermoelectric Material with Ultralow Lattice Thermal Conductivity and High Power Factor. **2018**, 30, 5639-5647	64
1169	General trends between solute segregation tendency and grain boundary character in aluminum - An ab inito study. **2018**, 158, 257-268	32
1168	Li doped kagome spin liquid compounds. **2018**, 20, 21693-21698	4
1167	Understanding the Intrinsic Surface Reactivity of Single-Layer and Multilayer PdO(101) on Pd(100). **2018**, 8, 8553-8567	31
1166	Unraveling the structure and bonding evolution of the newly discovered iron oxide FeO2. **2018**, 98,	51
1165	Discovery of High-Performance Thermoelectric Chalcogenides through Reliable High-Throughput Material Screening. **2018**, 140, 10785-10793	86
1164	Penta-PtN: an ideal two-dimensional material for nanoelectronics. **2018**, 10, 16169-16177	30
1163	Hierarchical mesoporous flower-like ZnCo2O4@NiO nanoflakes grown on nickel foam as high-performance electrodes for supercapacitors. **2018**, 284, 128-141	32
1162	From the Nonexistent Polar Intermetallic PtPr via PtPr to Pt/Sn/Pr Ternaries. **2018**, 57, 9949-9961	4
1161	New Calcium Hydrides with Mixed Atomic and Molecular Hydrogen. **2018**, 122, 19370-19378	27
1160	Lu5Pd4Ge8 and Lu3Pd4Ge4: Two More Germanides among Polar Intermetallics. **2018**, 8, 205	8
1159	The Crystal Orbital Hamilton Population (COHP) Method as a Tool to Visualize and Analyze Chemical Bonding in Intermetallic Compounds. **2018**, 8, 225	89
1158	Ba4[Mn3N6], a Quasi-One-Dimensional Mixed-Valent Nitridomanganate (II, IV). **2018**, 8, 235	2
1157	Structure and Chemical Bonding of the Li-Doped Polar Intermetallic RE□hLiGe□(RE = La, Nd, Sm, Gd; x = 0.13, 0.28, 0.43, 0.53) System. **2018**, 11,	2
1156	Insights into the Charge-Transfer Stabilization of Heterostructure Components with Unstable Bulk Analogs. **2018**, 30, 4738-4747	6
1155	Gold with +4 and +6 Oxidation States in AuF and AuF. **2018**, 140, 9545-9550	50
1154	Structural Diversity and Electronic Properties of 3d Transition Metal Tetraphosphides, TMP (TM = V, Cr, Mn, and Fe). **2018**, 57, 9385-9392	13

1153	Ultralow Overpotential of Hydrogen Evolution Reaction using Fe-Doped Defective Graphene: A Density Functional Study. **2018**, 10, 4450-4455	10
1152	Crystal and Magnetic Structures of the Chain Antiferromagnet CaFeAl. **2018**, 57, 5820-5829	2
1151	Hole Thermalization Dynamics Facilitate Ultrafast Spatial Charge Separation in CuFeO2 Solar Photocathodes. **2018**, 122, 11300-11304	22
1150	First Full Structural Characterization of Chloro Formamidinium Salts. **2018**, 644, 1485-1491	1
1149	Chemical composition and stress dependence of the elastic properties of □(Fe,Mn)3AlC thin films. **2018**, 153, 49-53	6
1148	Nonmetallic FeH6 under High Pressure. **2018**, 122, 12022-12028	21
1147	Low-frequency polarization in molecular-scale noble-metal/metal-oxide nanocomposites. **2018**, 10, 9583-9593	2
1146	Polyanionic Gold-Tin Bonding and Crystal Structure Preference in REAuSn (RE = La, Ce, Pr, Nd). **2018**, 57, 10736-10743	2
1145	Insights into Antibonding Induced Energy Density Enhancement and Exotic Electronic Properties for Germanium Nitrides at Modest Pressures. **2018**, 57, 10416-10423	2
1144	Direct Reaction of Nitrogen and Lithium up to 75 GPa: Synthesis of the LiN, LiN, LiN, and LiN Compounds. **2018**, 57, 10685-10693	23
1143	Insights into Different Products of Nitrosobenzene and Nitrobenzene Hydrogenation on Pd(111) under Realistic Reaction Conditions. **2018**, 122, 20337-20350	25
1142	The high reactive site and the unusually short Sc-C bond of the scandium phosphinoalkylidene complex, an explanation from first-principles calculation. **2018**, 118, e25691	
1141	Controlled Crystal Growth of Indium Selenide, InSe, and the Crystal Structures of □-InSe. **2018**, 57, 11775-11781	49
1140	Soft phonon modes from off-center Ge atoms lead to ultralow thermal conductivity and superior thermoelectric performance in n-type PbSe□.□eSe. **2018**, 11, 3220-3230	75
1139	Superconducting SrSnP with Strong Sn□P Antibonding Interaction: Is the Sn Atom Single or Mixed Valent?. **2018**, 30, 6005-6013	8
1138	Ab-initio study of oxygen vacancy stability in bulk and Cerium-doped lutetium oxyorthosilicate. **2018**, 204, 499-505	7
1137	First-Principles Study of the Adsorption and Depolymerization Mechanisms of Sodium Silicate on Iron Surfaces at High Temperature. **2018**, 122, 20827-20840	11
1136	Predicting the Electric Field Effect on the Lateral Interactions Between Adsorbates: O/Fe(100) from First Principles. **2018**, 61, 763-775	9

1135	Factors driving stable growth of He clusters in W: first-principles study. **2018**, 58, 076024	1
1134	Structural-Distortion-Driven Magnetic Transformation from Ferro- to Ferrimagnetic Iron Chains in B -based Nb FeIr B. **2018**, 57, 10323-10327	4
1133	Ternary palladium-indium-phosphorus and platinum-indium-phosphorus compounds based on the Cu3Au-type: Structure, bonding, and properties. **2018**, 265, 266-273	5
1132	Electronic Structure Analysis of the Diels-Alder Cycloaddition Catalyzed by Alkali-Exchanged Faujasites. **2018**, 122, 14733-14743	15
1131	Mesoporous NiCo2O4 nanoneedles@MnO2 nanoparticles grown on nickel foam for electrode used in high-performance supercapacitors. **2019**, 31, 167-177	26
1130	PySCF-NAO: An efficient and flexible implementation of linear response time-dependent density functional theory with numerical atomic orbitals. **2019**, 236, 188-204	7
1129	The electronic properties of hydrogenated Janus MoSSe monolayer: a first principles investigation. **2019**, 6, 105055	7
1128	Direct atomic insight into the role of dopants in phase-change materials. **2019**, 10, 3525	42
1127	Atomic Substitution to Balance Hardness, Ductility, and Sustainability in Molybdenum Tungsten Borocarbide. **2019**, 31, 7696-7703	8
1126	Lattice Expansion in Hybrid Perovskites: Effect on Optoelectronic Properties and Charge Carrier Dynamics. **2019**, 10, 5000-5007	38
1125	Grain-boundary corrosion of nickel-based alloy by synchrotron radiation technology. **2019**, 7, 278-283	2
1124	Phase-change heterostructure enables ultralow noise and drift for memory operation. **2019**, 366, 210-215	143
1123	Nitrogen-rich GaN5 and GaN6 as high energy density materials with modest synthesis condition. **2019**, 383, 125859	7
1122	Mechanism for unconventional nonlinear elasticity. **2019**, 100,	3
1121	From qualitative to quantitative description of the anomalous thermoelastic behavior of V, Nb, Ta, Pd and Pt. **2019**, 31, 225402	6
1120	Theoretical investigation of the valence states in Au via the Au-F compounds under high pressure. **2019**, 21, 17621-17627	5
1119	High-throughput computational discovery of In2Mn2O7 as a high Curie temperature ferromagnetic semiconductor for spintronics. **2019**, 5,	12
1118	Electronic structures of ultra-thin tellurium nanoribbons. **2019**, 11, 14134-14140	5

1117	Structure and Composition Modification of Ultrasmall Palladium Nanoparticles upon Hydrogenation from First Principles. **2019**, 123, 18609-18619	2
1116	Evaluating the Catalytic Efficiency of Paired, Single-Atom Catalysts for the Oxygen Reduction Reaction. **2019**, 9, 7660-7667	74
1115	Superior electrocatalytic hydrogen evolution at engineered non-stoichiometric two-dimensional transition metal dichalcogenide edges. **2019**, 7, 18357-18364	17
1114	Electronic and mechanical properties of predicted tin nitride stoichiometric compounds under high pressure. **2019**, 169, 109113	
1113	Scaling Relation of Oxygen Reduction Reaction Intermediates at Defective TiO2 Surfaces. **2019**, 123, 19486-19492	10
1112	Oxygen adsorption on the doped TiAl(1 0 0) surface. **2019**, 170, 109136	6
1111	Sn2Ga2S5: A Polar Semiconductor with Exceptional Infrared Nonlinear Optical Properties Originating from the Combined Effect of Mixed Asymmetric Building Motifs. **2019**, 31, 6268-6275	39
1110	Intrinsic and Extrinsic Defects in Layered Nitride Semiconductor SrTiN2. **2019**, 123, 19307-19314	5
1109	First-principles microkinetic study of methane and hydrogen sulfide catalytic conversion to methanethiol/dimethyl sulfide on Mo6S8 clusters: activity/selectivity of different promoters. **2019**, 9, 4573-4580	3
1108	Cation Clustering in Intermetallics: The Modular Bonding Schemes of CaCu and CaCu. **2019**, 58, 10313-10322	2
1107	Electronic Structure and Lithium Diffusion in LiAl(OH)Cl Studied by First Principle Calculations. **2019**, 24,	4
1106	The impact of vacancies on the stability of cubic phases in Sb□e binary compounds. **2019**, 11,	4
1105	DFT calculations in periodic boundary conditions of gas-phase acidities and of transition-metal anionic clusters: case study with carboxylate-stabilized ruthenium clusters. **2019**, 138, 1	3
1104	Five new ternary indium-arsenides discovered. Synthesis and structural characterization of the Zintl phases Sr3In2As4, Ba3In2As4, Eu3In2As4, Sr5In2As6 and Eu5In2As6. **2019**, 278, 120889	20
1103	Synthesis, crystal structure and physical properties of the solid solutions Ca14□REₓCdSb11 (RE = La□Nd, Sm, Gd□Yb, x □0.85 – 0.15). **2019**, 125, 245101	15
1102	The nature of Ni-O pairs for ethane activation on NiO(100) and NiO(110) surfaces. **2019**, 474, 110417	5
1101	Solving the Coloring Problem in Half-Heusler Structures: Machine-Learning Predictions and Experimental Validation. **2019**, 58, 9280-9289	11
1100	Designing ultrastrong 5d transition metal diborides with excellent stability for harsh service environments. **2019**, 21, 16095-16107	4

1099	The chemical nature of N doping on N doped carbon supported noble metal catalysts. **2019**, 375, 456-465	38
1098	SrPtIn- an orthorhombically distorted coloring variant of SrIn. **2019**, 48, 11411-11420	
1097	Understanding CrGeTe3: an abnormal phase change material with inverse resistance and density contrast. **2019**, 7, 9025-9030	17
1096	Structural and electronic properties of transition-metal chalcogenides Mo 5 S 4 nanowires. **2019**, 28, 106103	1
1095	Intrinsically Low Lattice Thermal Conductivity Derived from Rattler Cations in an AMM?Q3 Family of Chalcogenides. **2019**, 31, 8734-8741	15
1094	An omnidirectional visualization model of personalized gene regulatory networks. **2019**, 5, 38	7
1093	Synthesis and structure of Sr14Zn1+xAs11 and Eu14Zn1+xAs11 (x⁄0.5). New members of the family of pnictides isotypic with Ca14AlSb11, exhibiting a new type of structural disorder. **2019**, 280, 120990	14
1092	Revisiting Polytypism in Hexagonal Ternary Sulfide ZnIn2S4 for Photocatalytic Hydrogen Production Within the Z-Scheme. **2019**, 31, 9148-9155	30
1091	Understanding the Structure and Properties of Sesqui-Chalcogenides (i.e., V VI or Pn Ch (Pn = Pnictogen, Ch = Chalcogen) Compounds) from a Bonding Perspective. **2019**, 31, e1904316	57
1090	A neural network protocol for predicting molecular bond energy. **2019**, 62, 1698-1703	2
1089	Synthesis, Crystal and Electronic Structures, and Electrical Properties of the Fifth Member of the Rb(MoS)(MoS) Series: RbMoS, an Atypical Reduced Molybdenum Sulfide Containing Mo and Mo Clusters. **2019**, 58, 15236-15245	
1088	Effect of Impurities on the Oxygen Adsorption Properties on the NiTi(110) Surface. **2019**, 129, 413-420	
1087	Role of TM-TM Connection Induced by Opposite d-Electron States on the Hardness of Transition-Metal (TM = Cr, W) Mononitrides. **2019**, 58, 15573-15579	5
1086	XBi4S7 (X = Mn, Fe): New Cost-Efficient Layered n-Type Thermoelectric Sulfides with Ultralow Thermal Conductivity. **2019**, 29, 1904112	14
1085	Enhanced Iridium Mass Activity of 6H-Phase, Ir-Based Perovskite with Nonprecious Incorporation for Acidic Oxygen Evolution Electrocatalysis. **2019**, 11, 42006-42013	26
1084	Enhanced Interfacial H2 Activation for Nitrostyrene Catalytic Hydrogenation over Rutile Titania-Supported Gold by Coadsorption: A First-Principles Microkinetic Simulation Study. **2019**, 9, 11288-11301	11
1083	Exploring Chemical Bonding in Phase-Change Materials with Orbital-Based Indicators. **2019**, 13, 1800579	16
1082	Hydrogenation and structural properties of Mg100-2xLixAlx (x=12) limited solid solution. **2019**, 223, 503-511	8

1081	Largely Enhanced Seebeck Coefficient and Thermoelectric Performance by the Distortion of Electronic Density of States in GeSbTe. **2019**, 11, 34046-34052	19
1080	Unusually strong heteroatomic bonding in the complex polyanion of intermetallic BaPtAl. **2019**, 48, 14103-14114	
1079	Designing Multifunctionality via Assembling Dissimilar Materials: Epitaxial AlN/ScN Superlattices. **2019**, 123, 096801	7
1078	The influence of support materials on the structural and electronic properties of gold nanoparticles - a DFT study. **2019**, 21, 19011-19025	18
1077	Kinetically Controlled Low-Temperature Solid-State Metathesis of Manganese Nitride Mn3N2. **2019**, 31, 7248-7254	11
1076	Route to a Superconducting Phase above Room Temperature in Electron-Doped Hydride Compounds under High Pressure. **2019**, 123, 097001	125
1075	First-Principles Study of Piezoelectric Properties and Bonding Analysis in (Mg, X, Al)N Solid Solutions (X = Nb, Ti, Zr, Hf). **2019**, 4, 15081-15086	19
1074	Synthesis and Structure of a Nonstoichiometric ZrPtSb Compound. **2019**, 58, 12017-12024	1
1073	Hydrogenated PtP2 monolayer: theoretical predictions on the structure and charge carrier mobility. **2019**, 7, 12231-12239	9
1072	Electrostatic force driven helium insertion into ammonia and water crystals under pressure. **2019**, 2,	7
1071	Bifunctional N-CoSe2/3D-MXene as Highly Efficient and Durable Cathode for Rechargeable Zn–Air Battery. **2019**, 1, 432-439	49
1070	Revealing Electronic Signature of Lattice Oxygen Redox in Lithium Ruthenates and Implications for High-Energy Li-ion Battery Material Designs. **2019**, 31,	32
1069	LiZn: A Low Symmetric Polar Intermetallic Compound. **2019**, 58, 12590-12600	0
1068	Chemical Flexibility of Mg in Pnictide Materials: Structure and Properties Diversity. **2019**, 31, 8286-8300	9
1067	Identifying the Origins of Vacancies in the Crystal Structures of Rock Salt-type Chalcogenide Superconductors. **2019**, 4, 15721-15728	5
1066	Photomechanical effect leading to extraordinary ductility in covalent semiconductors. **2019**, 100,	6
1065	K2Ge3As3: Fiberlike Crystals of a Narrow-Band-Gap Zintl Phase with a One-Dimensional Substructure ∞1{(Ge3As3)2−} **2019**, 31, 8839-8849	3
1064	Predictions on High-Power Trivalent Metal Pentazolate Salts. **2019**, 10, 6166-6173	30

1063	Aluminum-silicon hydride clusters for prospective hydrogen storage. **2019**, 44, 26459-26468	2
1062	Quaternary rare-earth sulfides RE3M0.5M?S7 (M = Zn, Cd; M? = Si, Ge). **2019**, 278, 120914	4
1061	Vicinal metal surfaces as potential catalysts for phosphorene epitaxial growth. **2019**, 115, 113104	0
1060	New SbTeSe Monolayers with High Electron Mobilities and Wide Absorption Range. **2019**, 11, 37216-37228	7
1059	Prediction of improved magnetization and stability in Fe16N2 through alloying. **2019**, 126, 093903	10
1058	Electrical switching properties and structural characteristics of GeSe-GeTe films. **2019**, 11, 1595-1603	22
1057	Origin of high thermoelectric performance with a wide range of compositions for BiSbTe single quintuple layers. **2019**, 21, 1315-1323	6
1056	A hypervalent and cubically coordinated molecular phase of IF predicted at high pressure. **2019**, 10, 2543-2550	20
1055	Structure and Transport Properties in Itinerant Antiferromagnet RE(NiCu)AsO (RE = Ce, Sm). **2019**, 58, 2770-2776	2
1054	Elastic properties of the TiZrNbTaMo multi-principal element alloy studied from first principles. **2019**, 106, 130-140	12
1053	Electron density topological and adsorbate orbital analyses of water and carbon monoxide co-adsorption on platinum. **2019**, 150, 024703	6
1052	Electrocatalytic water oxidation over AlFeB. **2019**, 10, 2796-2804	31
1051	Fast Flux Reaction Approach for the Preparation of Sn2TiO4: Tuning Particle Sizes and Photocatalytic Properties. **2019**, 166, H3084-H3090	8
1050	First principles investigation into the phase stability and enhanced hardness of TiN-ScN and TiN-YN alloys. **2019**, 688, 137284	7
1049	Effects and distribution of Zr introduced in Ni-based cathode material for Li-ion batteries. **2019**, 21, 12505-12518	18
1048	Density functional study of methyl butanoate adsorption and its C-O bonds cleavage on MoS-based catalyst with various loads of Ni promoters. **2019**, 31, 365001	3
1047	Diversities of stoichiometry and electrical conductivity in sodium sulfides. **2019**, 7, 16472-16478	6
1046	Magnetostructural Coupling Drives Magnetocaloric Behavior: The Case of MnB versus FeB. **2019**, 31, 4873-4881	15

1045	Stability predictions of magnetic MAX compounds. **2019**, 31, 405902	11
1044	Synthesis and characterization of new quaternary polyselenide Ba4TMSbSe12 (TM = Nb, Ta). **2019**, 66, 1072-1077	
1043	Toward Heterolytic Bond Dissociation of Dihydrogen: The Study of Hydrogen in Arsenolite under High Pressure. **2019**, 123, 16868-16872	4
1042	First-principles explorations of Li2S@V2CTx hybrid structure as cathode material for lithium-sulfur battery. **2019**, 489, 677-683	19
1041	Indirect but Efficient: Laser-Excited Electrons Can Drive Ultrafast Polarization Switching in Ferroelectric Materials. **2019**, 10, 3402-3407	14
1040	Segregation of point defects at the CuInSe2(001)/GaAs(001) interface. **2019**, 299, 113652	1
1039	Stable zigzag and tripodal all-nitrogen anion N44□n BeN2. **2019**, 9, 055116	5
1038	Improving Performance of LiNi0.8Co0.1Mn0.1O2 Cathode Materials for Lithium-Ion Batteries by Doping with Molybdenum-Ions: Theoretical and Experimental Studies. **2019**, 2, 4521-4534	48
1037	Building Up a Picture of the Electrocatalytic Nitrogen Reduction Activity of Transition Metal Single-Atom Catalysts. **2019**, 141, 9664-9672	390
1036	Prediction of stable high-pressure structures of tantalum nitride TaN2. **2019**, 35, 2297-2304	5
1035	Revealing the Nature of Chemical Bonding in an ALn2Ag3Te5-Type Alkaline-Metal (A) Lanthanide (Ln) Silver Telluride. **2019**, 7, 70	7
1034	Equipartition of Energy Defines the Size-Thickness Relationship in Liquid-Exfoliated Nanosheets. **2019**, 13, 7050-7061	71
1033	Absolute energy level positions in tin- and lead-based halide perovskites. **2019**, 10, 2560	195
1032	Band-gap engineering in AB(OxS1□)3 perovskite oxysulfides: a route to strongly polar materials for photocatalytic water splitting. **2019**, 7, 15741-15748	19
1031	Spin-Polarized Current in Ferromagnetic Half-Metallic Transition-Metal Iodide Nanowires. **2019**, 123, 15717-15723	8
1030	Doping and biaxial deformation engineering the thermoelectric transport properties in selenium crystal. **2019**, 297, 34-38	2
1029	Origin of structural stability of ScH molecular nanowires and their chemical-bonding behavior: Correlation effects of the Sc 3d electrons. **2019**, 150, 184307	6
1028	Interface-tuned selective reductive coupling of nitroarenes to aromatic azo and azoxy: a first-principles-based microkinetics study. **2019**, 21, 12555-12565	6

1027	Quaternary Core-Shell Oxynitride Nanowire Photoanode Containing a Hole-Extraction Gradient for Photoelectrochemical Water Oxidation. **2019**, 11, 19077-19086	25
1026	Dynamic Frustrated Lewis Pairs on Ceria for Direct Nonoxidative Coupling of Methane. **2019**, 9, 5523-5536	25
1025	CaFe2Ge2 with square-planar iron layers □Closing a gap in the row of CaT2Ge2 (T = Mn□n). **2019**, 276, 368-375	0
1024	Metallic and anti-metallic properties of strongly covalently bonded energetic AlN nitrides. **2019**, 21, 12029-12035	8
1023	Pt-rich intermetallic APt8P2 (A´= Ca and La). **2019**, 798, 53-58	0
1022	Phase transition and anharmonicity in SnSe. **2019**, 10, 100093	27
1021	Novel MAB phases and insights into their exfoliation into 2D MBenes. **2019**, 11, 11305-11314	64
1020	Inducing half metallicity with alloying in Heusler Compound CoFeMnSb. **2019**, 31, 335702	2
1019	Ternary palladium □Group 12 metal compounds of the Pd5TlAs-type: A case study. **2019**, 276, 217-225	2
1018	Impurity influence on the oxygen adsorption on Ti3Al(0001) surface. **2019**, 487, 898-906	5
1017	Effect of Rare-Earth Metals Substitution for Ca on the Crystal Structure and Thermoelectric Properties of the Ca11□RExSb_{10}□ System. **2019**, 19, 3498-3508	8
1016	Covalent bonding versus total energy: On the attainability of certain predicted low-energy carbon allotropes. **2019**, 148, 151-158	6
1015	Chemical optimization towards superior electrocatalysis of Janus 1T-MoSX (X = O, Se, Te) for hydrogen evolution: Small composition tuning makes big difference. **2019**, 310, 153-161	6
1014	Sr[LiAlON]:Eu-A high performance red phosphor to brighten the future. **2019**, 10, 1824	162
1013	Thermoelectric transport properties of Ni-, Pd-, and Pt- doped skutterudites with S-filling as charge compensation. **2019**, 9, 045325	8
1012	The nature of the chemical bond in oxyanionic crystals based on QTAIM topological analysis of electron densities.. **2019**, 9, 12020-12033	14
1011	Zinc substituted MgH2 - a potential material for hydrogen storage applications. **2019**, 44, 13632-13646	3
1010	Band Gap Tuning in Bismuth Oxide Carbodiimide BiONCN. **2019**, 58, 6467-6473	16

1009	Chemical Design Principles for Cache-Type Sc$_3$Sb$_4$Te Phase-Change Memory Materials. **2019**, 31, 4008-4015	32
1008	High-Throughput Screening for Advanced Thermoelectric Materials: Diamond-Like ABX Compounds. **2019**, 11, 24859-24866	44
1007	New stoichiometric compounds of Au-Hg system under high pressure. **2019**, 31, 315402	
1006	Synthesis, structure, and properties of rare-earth germanium sulfide iodides RE3Ge2S8I (RE = La, Ce, Pr). **2019**, 274, 162-167	1
1005	Systematic Theoretical Study of Electronic Structures and Stability of Transition-Metal-Adsorbed Graphdiyne Clusters. **2019**, 123, 8843-8850	14
1004	Achieving band convergence by tuning the bonding ionicity in n-type Mg Sb. **2019**, 40, 1693-1700	41
1003	Tin, The Enabler-Hydrogen Diffusion into Ruthenium. **2019**, 9,	10
1002	Amphoteric behavior of hydrogen (H+1 and H^{-1}) in complex hydrides from van der Waals interaction-including ab initio calculations. **2019**, 7, 6228-6240	4
1001	Promoting nitrogen electroreduction to ammonia with bismuth nanocrystals and potassium cations in water. **2019**, 2, 448-456	404
1000	Catalytic Synthesis of Nitric Monoxide at the AlN(0001) Surface: Ab Initio Analysis. **2019**, 123, 10893-10906	3
999	Potential high-Tc superconductivity in CaYH12 under pressure. **2019**, 99,	53
998	IrF Molecular Crystal under High Pressure. **2019**, 141, 5409-5414	27
997	Structural and electronic properties of MoSI nanowires by newly proposed theoretical compositional ordering. **2019**, 9, 1222	5
996	First-principles Calculations of the Effects of Mn, Cr, and Ni on Hydrogen Diffusion in BCC, FCC, and HCP Fe. **2019**, 105, 231-239	2
995	Role of defects in tuning the adsorption of CO over graphene-supported Co13 cluster. **2019**, 481, 1080-1088	5
994	LiMgCuAl: a new ordered quaternary superstructure to the icosahedral T-Mg(Zn,Al) phase with fullerene-like Al cluster. **2019**, 75, 168-174	1
993	Surface Compositions of Pt$_3$Pd/Pd(111) Alloys in the Presence of O and OH during Oxygen Reduction Reaction: A First-Principles Study. **2019**, 88, 044802	0
992	New insights on the GeSeTe phase diagram from theory and experiment. **2019**, 75, 246-256	4

991	Anionic Doping and Cationic Site Preference in CaYbAlSbGe (x = 0.2, 0.5, 0.7): Origin of the Enhanced Seebeck Coefficient and the Structural Transformation. **2019**, 58, 5827-5836	8
990	Enhanced Nèl temperature in EuSnP under pressure. **2019**, 48, 5327-5334	3
989	Intermediate band insertion by group-IIIA elements alloying in a low cost solar cell absorber CuYSe2: A first-principles study. **2019**, 383, 1972-1976	6
988	Bonding heterogeneity and lone pair induced anharmonicity resulted in ultralow thermal conductivity and promising thermoelectric properties in n-type AgPbBiSe. **2019**, 10, 4905-4913	44
987	Direct Reaction between Copper and Nitrogen at High Pressures and Temperatures. **2019**, 10, 1109-1114	24
986	Crystal and electronic structure studies on transparent conducting nitrides A 3N2 (A = Mg, Zn and Sn) and Sn3N4. **2019**, 6, 055912	2
985	Revisiting Bond Breaking and Making in EuCo P : Where are the Electrons?. **2019**, 25, 5865-5869	4
984	How oxides affect the stretching modes of carbon monoxide adsorbed on Ni catalyst?. **2019**, 478, 1074-1080	3
983	Strain Effects on Oxygen Reduction Activity of Pr2NiO4 Caused by Gold Bulk Dispersion for Low Temperature Solid Oxide Fuel Cells. **2019**, 2, 1210-1220	9
982	Unique Phase Diagram and Superconductivity of Calcium Hydrides at High Pressures. **2019**, 58, 2558-2564	12
981	ReGaGe: Intermetallic Compound with Pronounced Covalency in the Bonding Pattern. **2019**, 58, 2822-2832	2
980	Thermodynamics and superconductivity of SxSe1⊠H3. **2019**, 99,	20
979	In Situ Measure of Intrinsic Bond Strength in Crystalline Structures: Local Vibrational Mode Theory for Periodic Systems. **2019**, 15, 1761-1776	19
978	SrNi2Si and BaNi2Si □New Layered Silicides with Fused Nickel Six-membered Rings in a Boat Conformation. **2019**, 645, 388-395	
977	Water adsorption on olivine(010) surfaces: Effect of alkali and transition metal cation doping. **2019**, 150, 044703	4
976	Crystal Structure and Bonding in Intermetallic Compounds. **2019**,	
975	Weyl nodes and magnetostructural instability in antiperovskite Mn3ZnC. **2019**, 7, 121104	2
974	A computational study of hydrogen doping induced metal-to-insulator transition in CaFeO, SrFeO, BaFeO and SmMnO. **2019**, 21, 25397-25405	5

973	High electrical conductivity in the epitaxial polar metals LaAuGe and LaPtSb. **2019**, 7, 121107	5
972	Synthesis of a two-dimensional organic-inorganic bismuth iodide metalate through in situ formation of iminium cations. **2019**, 55, 14725-14728	13
971	Achieving an Ultrahigh Power Factor in SbTeSe Monolayers via Valence Band Convergence. **2019**, 11, 46688-46695	8
970	Transition Metal Doping of Phase Change Materials: Atomic Arrangement of Cr-Doped Ge2Sb2Te5. **2019**, 123, 30640-30648	4
969	Insight into the structure and bonding of copper(I) iodide clusters and a cluster-based coordination polymer. **2019**, 43, 16176-16187	3
968	Development of a robust tool to extract Mulliken and Löwdin charges from plane waves and its application to solid-state materials.. **2019**, 9, 29821-29830	37
967	DFT study of Rh and Ti dimers decorating N-doped pyridinic and pyrrolic graphene for molecular and dissociative hydrogen adsorption. **2019**, 464, 243-254	17
966	Quaternary rare-earth transition-metal phosphides REMnCuP2 (RE = Y, La□Nd, Sm, Gd□Tm, Lu) with CaAl2Si2-type structure and a polymorph of LaMnCuP2 with BaCu2S2-type structure. **2019**, 269, 100-106	4
965	Understanding the Polymorphism of A4[(UO2)3(PO4)2O2] (A = Alkali Metals) Uranyl Phosphate Framework Structures. **2019**, 19, 966-975	5
964	Structures of quaternary chromium silicides revealed by a combination of resonant X-ray diffraction and ab initio calculations. **2019**, 105, 130-138	
963	A New Family of Two-Dimensional Topological Materials: CdX (X = F, Cl, Br, and I). **2019**, 13, 1800466	0
962	1T-MoS2 monolayer doped with isolated Ni atoms as highly active hydrogen evolution catalysts: A density functional study. **2019**, 469, 292-297	28
961	Half-metallicity in uranium intermetallics: crystal structure prediction of a high-pressure phase of UCo. **2019**, 31, 025501	0
960	Predicting pressure-stabilized alkali metal iridides: A□Ir (A = Rb, Cs). **2019**, 158, 124-129	5
959	Deriving bonding concepts for molecules, surfaces, and solids with energy decomposition analysis for extended systems. **2019**, 9, e1401	18
958	Hybridization-Switching Induced Mott Transition in ABO_{3} Perovskites. **2019**, 122, 016404	11
957	Operando Observations and First-Principles Calculations of Reduced Lithium Insertion in Au-Coated LiMn2O4. **2019**, 6, 1801923	9
956	Layered Bismuth Oxyfluoride Nitrates Revealing Large Second-Harmonic Generation and Photocatalytic Properties. **2019**, 58, 2183-2190	21

955	Hybrid porous flower-like NiO@CeO2microspheres with improved pseudocapacitiveproperties. **2019**, 297, 593-605	33
954	Correlations between Density-Based Bond Orders and Orbital-Based Bond Energies for Chemical Bonding Analysis. **2019**, 123, 2843-2854	23
953	Designing crystallization in phase-change materials for universal memory and neuro-inspired computing. **2019**, 4, 150-168	356
952	SrCdGeS4 and SrCdGeSe4: Promising Infrared Nonlinear Optical Materials with Congruent-Melting Behavior. **2019**, 19, 1206-1214	39
951	The BaS(VOS) Oxysulfide: One-Dimensional Structure and Mixed Anion Chemical Bonding. **2019**, 58, 1349-1357	4
950	Tuneable thermal expansion of poly (3,4-ethylenedioxythiophene) polystyrene sulfonate. **2019**, 31, 125101	3
949	Theoretical investigation on vanadium dinitrides from first-principles calculations. **2019**, 45, 2457-2465	5
948	Correlation between thermal-vibration-induced large displacement of Cu atoms and phase transition in Cu4SnS4: First-principles investigation. **2019**, 166, 37-46	3
947	Cationic Pb Dumbbells Stabilized in the Highly Covalent Lead Nitridosilicate Pb Si N. **2019**, 58, 1432-1436	9
946	Mechanistic Insight into the [4 + 2] Diels-Alder Cycloaddition over First Row d-Block Cation-Exchanged Faujasites. **2019**, 9, 376-391	7
945	The hardness mechanism and bonding properties of CrN2: A first principle study. **2019**, 158, 282-288	2
944	Predicted semiconducting beryllium sulfides in 3D and 2D configurations: Insights from first-principles calculations. **2019**, 781, 371-377	3
943	Capability of defective graphene-supported Co4 nanoparticle toward ammonia dehydrogenation. **2019**, 465, 1-9	7
942	Physicochemical, quantum mechanical and thermoanalytical investigations of newly synthesized pentakis(2,4-dimethylphenoxo) niobium (V) as potential precursor of Nb2O5. **2019**, 12, 5268-5277	1
941	Potentially Antibacterial Mixed-Ligand Oxidovanadium(IV) Salicylhydroxamate Complex [VO(acac)SHA]: Synthesis, Characterization and Quantum Mechanical Study. **2020**, 90, 213-223	0
940	Complex magnetic structure and related thermodynamic properties of Mn2SnS4. **2020**, 497, 165991	3
939	Predicting excellent anisotropic thermoelectric performance of the layered oxychalcogenides BiAgOCh (Ch = S, Se, and Te). **2020**, 171, 109273	4
938	Chalcogenide Thermoelectrics Empowered by an Unconventional Bonding Mechanism. **2020**, 30, 1904862	88

937	Local structure adaptability through multi cations for oxygen redox accommodation in Li-Rich layered oxides. **2020**, 24, 384-393	75
936	Construction of spherical NiO@MnO2 with core-shell structure obtained by depositing MnO2 nanoparticles on NiO nanosheets for high-performance supercapacitor. **2020**, 46, 421-429	29
935	Exploring the electronic structure and thermal properties of UAl3 using density functional theory calculations. **2020**, 136, 109179	2
934	Re-examining the nature of ordering in CaMnO2: The role of Mn-O covalency in the local structure. **2020**, 581, 411837	1
933	Discovery of space aromaticity in transition metal monoxide crystal Nb3O3 enabled by octahedral Nb6 structural units. **2020**, 65, 367-372	0
932	Electronic structure based design of thin film metallic glasses with superior fracture toughness. **2020**, 186, 108327	11
931	DFT study on H2 and H adsorption and the electronic properties of single atom Cu modified Fe (1 1 1) surface. **2020**, 505, 144526	3
930	Structural, mechanical and electronic properties study on group 5 transition metals ternary mononitrides from first-principles calculations. **2020**, 813, 152246	6
929	Review of Computational Studies of NCM Cathode Materials for Li-ion Batteries. **2020**, 60, 850-862	18
928	Insight into the magnetic moment of iron borides: theoretical consideration from the local coordinative and electronic environment. **2020**, 49, 2168-2175	2
927	The role of lattice vibration in the terahertz region for proton conduction in 2D metal-organic frameworks. **2019**, 11, 1538-1541	6
926	The Structural Stability of P2-Layered Na-Based Electrodes during Anionic Redox. **2020**, 4, 420-434	47
925	Isolated Boron Sites for Electroreduction of Dinitrogen to Ammonia. **2020**, 10, 1847-1854	82
924	The importance of the Mg Mg interaction in Mg3Sb2 Mg3Bi2 shown through cation site alloying. **2020**, 8, 2033-2038	18
923	Elucidating reaction equations of TiFx (x = 4,3,2) catalysts for hydrogen storage applications. **2020**, 45, 2818-2828	3
922	Two-Dimensional (001) LaAlO/SrTiO Heterostructures with Adjustable Band Gap and Magnetic Properties. **2020**, 12, 3134-3139	7
921	Unraveling the Structure-Valence-Property Relationships in AMM?Q3 Chalcogenides with Promising Thermoelectric Performance. **2020**, 3, 2110-2119	7
920	High-pressure X-ray diffraction and Mssbauer spectroscopy study of Fe1.087Te. **2020**, 578, 411875	

919	Site preference of V and its influence on the elastic properties in the boride series VxMo5−xSiB2 as studied by first principles density functional theory. **2020**, 819, 153041	2
918	Polymorphs, phase transitions and stability in BaM2(PO4)2 M = Mn, Fe, Co systems. **2020**, 7, 239-246	3
917	Strain-engineering enables reversible semiconductor–metal transition of skutterudite IrAs3. **2020**, 7, 1108-1114	1
916	Thermal, electronic and thermoelectric properties of TiNiSn and TiCoSb based quaternary half Heusler alloys obtained from ab initio calculations. **2020**, 4, 895-910	9
915	Charge-transfer descriptor for the cycle performance of Li2MO3 cathodes: role of oxygen dimers. **2020**, 8, 2663-2671	5
914	Lithium intercalation drives mechanical properties deterioration in bulk and single-layered black phosphorus: a first-principles study. **2020**, 7, 025028	5
913	Phase Transition from Weak Ferroelectricity to Incipient Ferroelectricity in Li2Sr(Nb1−xTax)2O7. **2020**, 32, 744-750	9
912	Layered Cathode Materials for Lithium-Ion Batteries: Review of Computational Studies on LiNi1−x−yCoxMnyO2 and LiNi1−x−yCoxAlyO2. **2020**, 32, 915-952	76
911	Designing Sulfide Borate as a Novel Type of Second-Order Nonlinear-Optical Material. **2020**, 59, 1547-1555	35
910	Understanding hydrogen in perovskites from first principles. **2020**, 174, 109461	8
909	Accelerating water dissociation kinetics on Ni3S2 nanosheets by P-induced electronic modulation. **2020**, 381, 493-500	20
908	Quantum-Chemical Study of the FeNCN Conversion-Reaction Mechanism in Lithium- and Sodium-Ion Batteries. **2020**, 59, 3718-3723	14
907	Zintl phase crystal assembled by magic Al6CNa4 cluster. **2020**, 739, 137026	
906	Exploring the Origins of Improved Photocurrent by Acidic Treatment for Quaternary Tantalum-Based Oxynitride Photoanodes on the Example of CaTaO2N. **2020**, 124, 152-160	20
905	Fe5−xGe2Te2: New Exfoliable Itinerant Ferromagnet with High Curie Temperature and Large Perpendicular Magnetic Anisotropy. **2020**, 14, 1900666	4
904	Facile CO Oxidation on Oxygen-functionalized MXenes via the Mars-van Krevelen Mechanism. **2020**, 12, 1007-1012	2
903	Tungsten as "Adhesive" in Pt2CuW0.25 Ternary Alloy for Highly Durable Oxygen Reduction Electrocatalysis. **2020**, 30, 1908230	32
902	Theoretical study on structural, mechanical and electronic properties of ternary mononitride Ti0.5W0.5N from first-principles calculations. **2020**, 242, 122476	4

901	New group V graphyne: two-dimensional direct semiconductors with remarkable carrier mobilities, thermoelectric performance, and thermal stability. **2020**, 12, 100164	7
900	Localized dimers drive strong anharmonicity and low lattice thermal conductivity in ZnSe2. **2020**, 102,	4
899	First Principles Density Functional Theory Prediction of the Crystal Structure and the Elastic Properties of Mo2ZrB2 and Mo2HfB2. **2020**, 10, 865	0
898	Revealing the Bonding Nature in an ALnZnTe3-Type Alkaline-Metal (A) Lanthanide (Ln) Zinc Telluride by Means of Experimental and Quantum-Chemical Techniques. **2020**, 10, 916	4
897	Bi-Doped Zirconium Alloys with Enhanced Water Oxidation Resistance. **2020**, 124, 23116-23125	0
896	Tunable Luminescence in Hybrid Cu(I) and Ag(I) Iodides. **2020**, 59, 15487-15494	3
895	Prediction of Highly Selective Electrocatalytic Nitrogen Reduction at Low Overpotential on a Mo-Doped g-GaN Monolayer. **2020**, 10, 12841-12857	37
894	Role of Hydrogen-Bonding and OH-□Interactions in the Adhesion of Epoxy Resin on Hydrophilic Surfaces. **2020**, 5, 26211-26219	12
893	Vacancy-Induced Oxygen Reduction Activity in Janus Transition Metal Dichalcogenides. **2020**, 7, 4233-4238	2
892	Stability and bonding nature of tin borohydride. **2020**, 45, 23103-23111	
891	Enhanced electrochemical oxygen evolution reaction activity on natural single-atom catalysts transition metal phthalocyanines: the substrate effect. **2020**, 10, 8339-8346	8
890	A new carbon allotrope: T5-carbon. **2020**, 189, 72-77	6
889	Ferroelectricity and phase transitions in InSe van der Waals material. **2020**, 12, 22688-22697	8
888	Ca14AlBi11□ new Zintl phase from earth-abundant elements with a great potential for thermoelectric energy conversion. **2020**, 7, 100094	8
887	Mechanistic Understanding on the Role of Cu Species over the CuO /TiO Catalyst for CO Photoreduction. **2020**, 5, 18050-18063	6
886	Exploring the sub-stoichiometric behavior of plutonium mononitride.. **2020**, 10, 24877-24881	1
885	Theoretical and Experimental Insights into the Effects of Zn Doping on the Magnetic and Magnetocaloric Properties of MnCoGe. **2020**, 32, 6721-6729	2
884	Molybdenum defect complexes in bismuth vanadate. **2020**, 22, 16277-16285	1

883	Thermoelectric transport of semiconductor full-Heusler VFe2Al. **2020**, 8, 10174-10184	15
882	3D branched rutile TiO2 @ rutile SnO2 nanorods array heteroarchitectures/carbon cloth with an adjustable band gap to enhance lithium storage reaction kinetics for flexible lithium-ion batteries. **2020**, 354, 136727	13
881	The contrasting fracture behaviour of twin boundaries and general boundaries A first principles study based on experimental observation. **2020**, 781, 139225	5
880	Atom-Pair Catalysts Supported by N-Doped Graphene for the Nitrogen Reduction Reaction: -Band Center-Based Descriptor. **2020**, 11, 6320-6329	40
879	Enhancing the Stability of Orthorhombic CsSnI Perovskite Oriented Conjugated Ligand Passivation. **2020**, 12, 34462-34469	11
878	Binary Intermetallics in the 70 atom % R Region of Two R-Pd Systems (R = Tb and Er): Hidden, Obscured, or Nonexistent?. **2020**, 59, 10802-10812	2
877	Improving Stability of Lead Halide Perovskite via PbF Layer Covering. **2020**, 11, 6266-6272	7
876	Trends in Alkaline Hydrogen Evolution Activity on Cobalt Phosphide Electrocatalysts Doped with Transition Metals. **2020**, 1, 100136	20
875	Origin of magnetic phase transition in RMn2Si2 (R = rare-earth ion or Y) intermetallics. **2020**, 184, 109901	1
874	Photoexcitation Induced Ultrafast Nonthermal Amorphization in SbTe. **2020**, 11, 10242-10249	5
873	Copper(I)-Based Flexible Organic-Inorganic Coordination Polymer and Analogues: High-Power Factor Thermoelectrics. **2020**,	5
872	Achieving high hydrogen evolution reaction activity of a MoC monolayer. **2020**, 22, 26189-26199	4
871	Ligand Stabilized Ni Catalyst for Efficient CO Oxidation. **2020**, 21, 2417-2425	2
870	Atomistic and Electronic Origin of Phase Instability of Metal Halide Perovskites. **2020**, 3, 11548-11558	16
869	Hydrogen Pentagraphenelike Structure Stabilized by Hafnium: A High-Temperature Conventional Superconductor. **2020**, 125, 217001	31
868	Direct Correlation of Mechanical Hardness and Chemical Bonding in Intermetallic Double Perovskite Borides Sc2Ir6PdxB. **2020**, 124, 26062-26067	2
867	Active learning for the power factor prediction in diamond-like thermoelectric materials. **2020**, 6,	12
866	The effect of the elements Cr, Os, Ir, and Y additions on the mechanical and electronic properties of L12 Ni3Co alloys. **2020**, 128, 185110	2

865	Arsenic adsorption on hematite facets: spectroscopy and DFT study. **2020**, 7, 3927-3939	15
864	Single transition metal atoms on nitrogen-doped carbon for CO2 electrocatalytic reduction: CO production or further CO reduction?. **2020**, 533, 147466	21
863	Quaternary Arsenides REHfCuAs (RE = La-Nd; □□0.17): Superstructures of the ZrNiP-Type Structure. **2020**, 59, 11089-11095	2
862	Large lattice thermal conductivity, interplay between phonon-phonon, phonon-electron, and phonon-isotope scatterings, and electrical transport in molybdenum from first principles. **2020**, 102,	4
861	The partition principles for atomic-scale structures and their physical properties: application to the nonlinear optical crystal material KBeBOF. **2020**, 22, 19299-19306	3
860	Molybdenum carbide nano-sheet as a high capacity anode material for monovalent alkali metal-ion batteries□theoretical investigation. **2020**, 384, 126688	1
859	Electronic Structure Based Intuitive Design Principle of Single-Atom Catalysts for Efficient Electrolytic Nitrogen Reduction. **2020**, 12, 5456-5464	10
858	Exceptional plasticity in the bulk single-crystalline van der Waals semiconductor InSe. **2020**, 369, 542-545	60
857	Correlating C?C, C?O, and C?N Hydrogenation Activity with Hydrogen Binding Energies on Ni□e Bimetallic Catalysts. **2020**, 124, 18595-18603	1
856	Hydrogen in Nanocatalysis. **2020**, 11, 7049-7057	10
855	Analysis and assessment of the structural, electronic properties of (ZrH2)n (n´=´5□4) clusters: Density function theory calculations. **2020**, 1188, 112940	2
854	Tackling the Inertness of CO2: Facile Activation and Electroreduction on the Metal-Free SiN4C4 Monolayer Sheet. **2020**, 124, 18660-18669	6
853	New cubic cluster phases in the Mg-Ni-Ga system. **2020**, 76, 534-542	1
852	A multi-scale simulation of syngas combustion reactions by Ni-based oxygen carriers for chemical looping combustion. **2020**, 531, 147277	11
851	Unveiling the structural origin to control resistance drift in phase-change memory materials. **2020**, 41, 156-176	34
850	Machine learning driven simulated deposition of carbon films: From low-density to diamondlike amorphous carbon. **2020**, 102,	20
849	High-Capacity Li+ Storage through Multielectron Redox in the Fast-Charging Wadsley□oth Phase (W0.2V0.8)3O7. **2020**, 32, 9415-9424	3
848	Assessment of PBE+U and HSE06 methods and determination of optimal parameter U for the structural and energetic properties of rare earth oxides. **2020**, 153, 164710	5

847	A thermodynamic and kinetic study of the catalytic performance of Fe, Mo, Rh and Ru for the electrochemical nitrogen reduction reaction. **2020**, 22, 25973-25981	4
846	Octahedral morphology of NiO with (111) facet synthesized from the transformation of NiOHCl for the NOx detection and degradation: experiment and DFT calculation. **2020**, 7, 3431-3442	7
845	Pore-Edge Tailoring of Single-Atom Iron–Nitrogen Sites on Graphene for Enhanced CO2 Reduction. **2020**, 10, 10803-10811	62
844	Elucidating Mechanistic Origin of the Catalytic Activity of the Fe(111) Surface and Nanoclusters toward the Electrochemical Nitrogen Reduction Reaction. **2020**, 124, 20193-20202	3
843	Structural characterization and property modification for two-dimensional (001) SrTiO3 nanosheets. **2020**, 10, 4273-4279	2
842	Atomic-Scale Insights into Emergent Photovoltaic Absorbers. **2020**,	
841	SnCN2: A Carbodiimide with an Innovative Approach for Energy Storage Systems and Phosphors in Modern LED Technology. **2020**, 7, 4550-4561	7
840	Chemistry under high pressure. **2020**, 4, 508-527	43
839	Hierarchical Contribution of Anions to Second Harmonic Generation in A2HgI4 (A = Na, Ag, Cu) Regulated Dramatically by Metal Cations. **2020**, 20, 7470-7476	1
838	Density Functional Theory Calculations of the Stability and Statistical Disorder in Crystals of the Kappa Phase of Me3 + xW10 − xC3 + y (Me = Fe, Co, Ni). **2020**, 94, 1369-1374	
837	Screening a Suitable Mo Form Supported on Graphdiyne for Effectively Electrocatalytic N Reduction Reaction: From Atomic Catalyst to Cluster Catalyst. **2020**, 11, 8128-8137	30
836	Composition-Gradient-Mediated Semiconductor-Metal Transition in Ternary Transition-Metal-Dichalcogenide Bilayers. **2020**, 12, 45184-45191	5
835	Insights into Syngas Combustion on a Defective NiO Surface for Chemical Looping Combustion: Oxygen Migration and Vacancy Effects. **2020**, 124, 28359-28370	8
834	Three-site transition-metal clusters: Going from localized electrons to molecular orbitals. **2020**, 102,	3
833	Silver Cyanoguanidine Nitrate Hydrate: Ag(C2N4H4)NO3 · H2O, a Cyanoguanidine Compound Coordinating by an Inner Nitrogen Atom. **2020**, 8, 64	0
832	Theoretical investigation on graphene-supported single-atom catalysts for electrochemical CO2 reduction. **2020**, 10, 8465-8472	11
831	Boron Concentration Induced Co-Ta-B Composite Formation Observed in the Transition from Metallic to Covalent Glasses. **2020**, 5, 18	
830	Mixed metal oxide: A new class of catalyst for methanol activation. **2020**, 534, 147449	2

829	Effect of the Free Volume on the Electronic Structure of CuZr Metallic Glasses. **2020**, 13,	1
828	Structural Evolution and Magnetic Properties of GdHfO Nanocrystals: Computational and Experimental Investigations. **2020**, 25,	2
827	Interplay of covalency, non-cubic crystal field, and spin-orbit coupling: A comparative study of d5,d4, and d3 double perovskite iridates Sr2MIrO6 (M = Ce, Sc, Ca). **2020**, 507, 166827	1
826	Effect of chemical composition, defect structure, and stress state on the elastic properties of (V Al)N. **2020**, 32, 025901	4
825	Origin of Confined Catalysis in Nanoscale Reactors between Two-Dimensional Covers and Metal Substrates: Mechanical or Electronic?. **2020**, 124, 11564-11573	8
824	Predicting Spinel Disorder and Its Effect on Oxygen Transport Kinetics in Hercynite. **2020**, 12, 23831-23843	5
823	Synthesis, Structural Characterization and Chemical Bonding of Sr7Li6Sn12 and its Quaternary Derivatives with Eu and Alkaline Earth Metal (Mg, Ca, Ba) Substitutions. A Tale of Seven Li-Containing Stannides and Two Complex Crystal Structures. **2020**, 2020, 1979-1988	
822	Kinetically Limited Phase Formation of Pt-Ir Based Compositionally Complex Thin Films. **2020**, 13,	1
821	A quantum chemical study of substituent effects on CN bonds in aryl isocyanide molecules adsorbed on the Pt surface. **2020**, 22, 12200-12208	2
820	Superconducting boron allotropes. **2020**, 101,	8
819	Electronic, optical, and thermoelectric properties of sodium pnictogen chalcogenides: A first principles study. **2020**, 183, 109818	8
818	Computational prediction of a +4 oxidation state in Au via compressed AuO compound. **2020**, 32, 015402	0
817	Role of surface frustrated Lewis pairs on reduced CeO2(110) in direct conversion of syngas. **2020**, 41, 1906-1915	16
816	Crystal structure and physical properties of AePd1-xP1+x (Ae = Ca, Sr). **2020**, 25, 101284	
815	Moderate Pressure Stabilized Pentazolate Cyclo-N Anion in Zn(N) Salt. **2020**, 59, 8002-8012	15
814	Probing the Validity of the Zintl-Klemm Concept for Alkaline-Metal Copper Tellurides by Means of Quantum-Chemical Techniques. **2020**, 13,	4
813	Elucidation of the Active Sites for Monodisperse FePt and Pt Nanocrystal Catalysts for p-WSe2 Photocathodes. **2020**, 124, 11877-11885	5
812	Transfer Hydrogenation of Cinnamaldehyde Catalyzed by Al2O3 Using Ethanol as a Solvent and Hydrogen Donor. **2020**, 8, 8195-8205	9

811	Synthesis, electronic structure and physical properties of two new layered compounds, EuFAgSe and EuFAgTe, featuring the active redox pair Eu/Ag. **2020**, 49, 7426-7435	1
810	The Microstructure and Electronic Properties of Yttrium Oxide Doped With Cerium: A Theoretical Insight. **2020**, 8, 338	2
809	Atomically embedded asymmetrical dual-metal dimers on N-doped graphene for ultra-efficient nitrogen reduction reaction. **2020**, 388, 77-83	66
808	Interdependence of Oxygenation and Hydration in Mixed-Conducting (Ba,Sr)FeO3 Perovskites Studied by Density Functional Theory. **2020**, 124, 11780-11789	12
807	Chemical Bonding in Chalcogenides: The Concept of Multicenter Hyperbonding. **2020**, 32, e2000340	21
806	Recent Studies on the Nature and State of Carbon Atoms in Iron. **2020**, 106, 331-341	1
805	Linear scaling relations for N2H4 decomposition over transition metal catalysts. **2020**, 45, 16114-16121	3
804	Rare-earth Metal Borosilicides R9Si15B3 (R = Tb, Yb): New Ordered Structures Derived from the AlB2 Structure Type. **2020**, 646, 1168-1175	0
803	Synthesis and structural characterization of the new Zintl phases Ba3Cd2P4 and Ba2Cd2P3. Rare example of small gap semiconducting behavior with negative thermopower within the range 300 K 00 K. **2020**, 289, 121476	9
802	Chemical bonding analysis in Ti1 yAlxTayN solid solutions. **2020**, 395, 125802	4
801	Tuning Single-Atom Catalysts of Nitrogen-Coordinated Transition Metals for Optimizing Oxygen Evolution and Reduction Reactions. **2020**, 124, 13168-13176	14
800	Rational Design of a NiN Electrocatalyst to Accelerate Polysulfide Conversion in Lithium-Sulfur Batteries. **2020**, 14, 6673-6682	103
799	Strain effect on the catalytic activities of B- and B/N-doped black phosphorene for electrochemical conversion of CO to valuable chemicals. **2020**, 8, 11986-11995	12
798	Siesta: Recent developments and applications. **2020**, 152, 204108	69
797	Physical properties of 2D MXenes: from a theoretical perspective. **2020**, 3, 032006	15
796	Crystal Structure and Electronic Properties of New Compound ZrPtSe. **2020**, 59, 8196-8202	
795	The MAX phase borides Zr2SB and Hf2SB. **2020**, 106, 106316	19
794	Unusual crystallographic ordering of two neighbouring elements - Cd and In in Cd2Cu3In, the first example in ternary Laves phase. **2020**, 844, 156054	3

793	On the New Oxyarsenides Eu5Zn2As5O and Eu5Cd2As5O. **2020**, 10, 475	0
792	Nitrogen reduction reaction on small iron clusters supported by N-doped graphene: A theoretical study of the atomically precise active-site mechanism. **2020**, 13, 2280-2288	22
791	A new monoclinic structure type for ternary gallide MgCoGa. **2020**, 76, 541-546	1
790	Does Spinel Serve as a Rigid Framework for Oxygen Redox?. **2020**, 32, 7181-7187	1
789	On the behaviour of structure-sensitive reactions on single atom and dilute alloy surfaces. **2020**, 10, 5815-5828	5
788	Chemical substitution of Zn in the structure of ordered Cu6Zn2Sb2: A structural and theoretical study. **2020**, 107, 106333	2
787	LOBSTER: Local orbital projections, atomic charges, and chemical-bonding analysis from projector-augmented-wave-based density-functional theory. **2020**, 41, 1931-1940	155
786	Unique 2D–3D Structure Transformations in Trichalcogenide CrSiTe3 under High Pressure. **2020**, 124, 15600-15606	5
785	Mechanism of selective and complete oxidation in La2O3-catalyzed oxidative coupling of methane. **2020**, 10, 2602-2614	14
784	First-Principles Investigation of β-FeOOH for Hydrogen Evolution: Identifying Reactive Sites and Boosting Surface Reactions. **2020**, 26, 7118-7123	3
783	Decoupling electrolytes towards stable and high-energy rechargeable aqueous zinc–manganese dioxide batteries. **2020**, 5, 440-449	203
782	Heterostructured CoP/MoO2 on Mo foil as high-efficiency electrocatalysts for the hydrogen evolution reaction in both acidic and alkaline media. **2020**, 8, 6732-6739	38
781	The influence of oxygen vacancy and Ce3+ ion positions on the properties of small gold clusters supported on CeO2−x(111). **2020**, 8, 15695-15705	8
780	Metal-rich tellurides PdTe1−xBix as functional materials: Catalytic behavior in the Fischer–Tropsch synthesis and bonding analysis. **2020**, 13, 2041001	1
779	A new ternary silicide GdFe1−xSi2 (x=0.32): preparation, crystal and electronic structure. **2020**, 75, 217-223	1
778	Pressure-induced non-innocence in bis(1,2-dionedioximato)Pt(ii) complexes: an experimental and theoretical study of their insulator-metal transitions. **2020**, 22, 6677-6689	5
777	First-principles investigations of orthorhombic-cubic phase transition and its effect on thermoelectric properties in cobalt-based ternary alloys. **2020**, 32, 055505	5
776	Pressure-Stabilized Zinc Trifluoride. **2020**, 11, 2854-2858	4

775	In Situ Assessment of Intrinsic Strength of X-I?OA-Type Halogen Bonds in Molecular Crystals with Periodic Local Vibrational Mode Theory. **2020**, 25,	19
774	High Thermoelectric Performance in Sulfide-Type Argyrodites Compound Ag8Sn(S1⊠Sex)6 Enabled by Ultralow Lattice Thermal Conductivity and Extended Cubic Phase Regime. **2020**, 30, 2000526	17
773	Unraveling the role of bonding chemistry in connecting electronic and thermal transport by machine learning. **2020**, 8, 8716-8721	9
772	Revealing the oxygen reduction reaction activity origin of single atoms supported on g-C3N4 monolayers: a first-principles study. **2020**, 8, 6555-6563	57
771	Surface Strain-Induced Collective Switching of Ensembles of Molecules on Metal Surfaces. **2020**, 11, 2277-2283	3
770	Properties and Structural Arrangements of the Electrode Material CuDEPP during Energy Storage. **2020**, 8, 2000388	
769	Crystal Orbital Overlap Population and X-ray Absorption Spectroscopy. **2020**, 124, 6111-6118	6
768	Localized High Concentration Electrolytes for High Voltage Lithium⊠Metal Batteries: Correlation between the Electrolyte Composition and Its Reductive/Oxidative Stability. **2020**, 32, 5973-5984	41
767	Pressure-Induced Superconductivity in the Wide-Band-Gap Semiconductor Cu2Br2Se6 with a Robust Framework. **2020**, 32, 6237-6246	4
766	Pairing of Transition Metal Dichalcogenides and Doped Graphene for Catalytically Dual Active Interfaces for the Hydrogen Evolution Reaction. **2020**,	
765	Site preference and atomic ordering in the structure of In3Pd5: A theoretical study. **2020**, 290, 121567	2
764	Phase Engineering of Transition Metal Dichalcogenides with Unprecedentedly High Phase Purity, Stability, and Scalability via Molten-Metal-Assisted Intercalation. **2020**, 32, e2001889	24
763	Contrasting SnTe-NaSbTe and SnTe-NaBiTe Thermoelectric Alloys: High Performance Facilitated by Increased Cation Vacancies and Lattice Softening. **2020**, 142, 12524-12535	21
762	Tailoring the Mechanical Properties of Earth-Abundant Transition Metal Borides via Bonding Optimization. **2020**, 124, 4430-4437	5
761	Bonding similarities and differences between Y⊠bTe and Sc⊠bTe phase-change memory materials. **2020**, 8, 3646-3654	21
760	Copper halide diselenium: predicted two-dimensional materials with ultrahigh anisotropic carrier mobilities.. **2020**, 10, 8016-8026	5
759	Molecular chemisorption of N on IrO(110). **2020**, 152, 074712	10
758	Tuning of interactions between cathode and lithium polysulfide in Li-S battery by rational halogenation. **2020**, 49, 147-152	10

757	Quantum-Chemical Study of the FeNCN Conversion-Reaction Mechanism in Lithium- and Sodium-Ion Batteries. **2020**, 132, 3747-3752	2
756	Guided patchwork kriging to develop highly transferable thermal conductivity prediction models. **2020**, 3, 024006	8
755	A perspective on conventional high-temperature superconductors at high pressure: Methods and materials. **2020**, 856, 1-78	132
754	Study of nontrivial magnetism in 3d□d transition metal based double perovskites. **2020**, 101,	3
753	New Findings on an Old Question: Can Defect-Free Graphene Monolayers be Superior Metal-Ion Battery Anodes?. **2020**, 4, 1900152	7
752	Local removal of silicon layers on Si(1′0′0)-2□1 with chlorine-resist STM lithography. **2020**, 509, 145235	9
751	Electronic effects of transition metal dopants on Fe(100) and Fe5C2(100) surfaces for CO activation. **2020**, 10, 2047-2056	5
750	CO2 Adsorptions on d-Block-Metal-Doped Nickel Nanoparticles: Unexpected Adsorption Configurations Predicted by Machine Intelligence. **2021**, 125, 19839-19846	0
749	Two-Dimensional Janus FeXY (X, Y = Cl, Br, and I, X □Y) Monolayers: Half-Metallic Ferromagnets with Tunable Magnetic Properties under Strain. **2021**, 13, 38897-38905	23
748	Insight into the Temperature Evolution of Electronic Structure and Mechanism of Exchange Interaction in EuS. **2021**, 12, 8328-8334	1
747	Density Functional Theory for Electrocatalysis.	12
746	Synthesis of calcium polysulfides at high pressures. **2021**, 104,	0
745	Boridene: Two-dimensional MoB with ordered metal vacancies obtained by chemical exfoliation. **2021**, 373, 801-805	22
744	New Compounds and Phase Selection of Nickel Sulfides via Oxidation State Control in Molten Hydroxides. **2021**, 143, 13646-13654	1
743	Orbital-scale understanding on high-selective hydrogenation of acetylene over Pt1-Cu(1 1 1) catalyst. **2021**, 240, 116664	2
742	Crystal and Electronic Structure Modification of Synthetic Perryite Minerals: A Facile Phase Transformation Strategy to Boost the Oxygen Evolution Reaction. **2021**, 60, 13607-13614	1
741	Mineralization of norfloxacin in a CoFe□DH/CF cathode-based heterogeneous electro-fenton system: Preparation parameter optimization of the cathode and conversion mechanisms of H2O2 to □OH. **2021**, 417, 129240	18
740	Structural, electronic and magnetic properties of TlFeSeunder high pressure. **2021**, 33,	

739	The strain and transition metal doping effects on monolayer Cr2O3 for hydrogen evolution reaction: The first principle calculations. **2021**,	0
738	Computational Study of the Effect of Doping with Ti on NaAlH4 Nanocluster Dehydrogenation. **2021**, 95, 1646-1654	
737	CO2 Hydrogenation on NixMg1−xAl2O4: A Comparative Study of MgAl2O4 and NiAl2O4. **2021**, 11, 1026	1
736	NiTe Monolayer: Two-Dimensional Metal with Superior Basal-Plane Activity for the Oxygen Reduction Reaction. **2021**, 125, 19164-19170	3
735	Transition metal atoms (Fe, Co, Ni, Cu, Zn) doped RuIr surface for the hydrogen evolution reaction: A first-principles study. **2021**, 556, 149801	7
734	Influence of vacancy on helium interaction with α-Zirconium. **2021**, 1989, 012039	
733	Mediating the Local Oxygen-Bridge Interactions of Oxysalt/Perovskite Interface for Defect Passivation of Perovskite Photovoltaics. **2021**, 13, 177	9
732	Exploring the anchoring effect and catalytic mechanism of 3d transition metal phthalocyanine for S8/LiPSs: A density functional theory study. **2021**, 558, 149928	2
731	Synthesis, Crystal Structure, Symmetry Relationships, and Electronic Structure of Bismuth Carbodiimide Bi(NCN) and Its Ammonia Adduct Bi(NCN)·NH. **2021**, 60, 12664-12670	2
730	Sr7N2Sn3: a layered antiperovskite-type nitride stannide containing zigzag chains of Sn4 polyanions. **2021**,	
729	Structural features of chalcogenide glass SiTe: An ovonic threshold switching material. **2021**, 9, 081101	4
728	Antibonding-Induced Anomalous Temperature Dependence of the Band Gap in Crystalline Ge2Sb2Te5. **2021**, 125, 19537-19543	2
727	Novel rubidium polyfluorides with F3, F4, and F5 species*. **2021**, 30, 066102	
726	Room-Temperature Ferroelectricity in 2D Metal-Tellurium-Oxyhalide CdTeClO Selenium-Induced Selective-Bonding Growth. **2021**, 15, 16525-16532	3
725	Theoretical Insights on Au-based Bimetallic Alloy Electrocatalysts for Nitrogen Reduction Reaction with High Selectivity and Activity. **2021**, 14, 4525-4535	1
724	Crystal and electronic structure of the new ternary phosphide Ho5Pd19P12. **2021**,	0
723	Lead-Free Halide CsPtI Perovskite Favoring Pt-N Bonding for Trace NO Detection. **2021**, 6, 3800-3807	1
722	Associative vs. dissociative mechanism: Electrocatalysis of nitric oxide to ammonia. **2021**, 33, 1051-1051	24

721	Role of facet in the competitive pathway of ethylene epoxidation. **2021**, 716, 121954	0
720	Lost horses on the frontier: K2BiCl5 and K3Bi2Br9. **2021**, 122621	
719	Orbital-selective electronic excitation in phase-change memory materials: a brief review. **2021**,	
718	Microstructural, electronic, and mechanical properties of Al4La and Al4Sm intermetallics: An experimental and first-principles calculations. **2021**, 616, 412853	1
717	Unravelling the crystal structure and optoelectronic properties of C3H3MI3 (M = Sn, Pb) for solar cell applications. **2021**, 230, 111133	0
716	Electronic Structure and Superconductivity of Compressed Metal Tetrahydrides. **2021**, 27, 14858-14870	3
715	How to Look for Compounds: Predictive Screening and in situ Studies in Na-Zn-Bi System. **2021**, 27, 15954-15966	6
714	Cd additive effect on self-flux growth of Cs-intercalated NbS2 superconducting single crystals. **2021**,	
713	A novel high-pressure phase of ScNwith higher stability predicted from first-principles calculations. **2021**, 33,	0
712	First-Principle Study of Co-Adsorption Behavior of H2O and O2 on δ-Pu (100) Surface. **2021**, 11, 1098	0
711	Lessons learned from FeSb2O4 on stereoactive lone pairs as a design principle for anion insertion. **2021**, 100592	1
710	Synthesis, crystal and electronic structure of CaNi2Al8. **2021**,	1
709	Electrocatalytic Hydrogen Evolution Reaction of Rhenium Metal and Rhenium-Based Intermetallic in Acid and Alkaline Media.	0
708	Synthesis, structure, and magnetic properties of the quaternary oxysulfides Ln5V3O7S6 (Ln = La, Ce). **2021**,	
707	Trace Iridium as ?Adhesive? in PtCuIr Aerogels for Robust Methanol Electrooxidation. **2021**, 9, 13039-13046	1
706	Engineering d-p Orbital Hybridization in Single-Atom Metal-Embedded Three-Dimensional Electrodes for Li-S Batteries. **2021**, 33, e2105947	41
705	Exploring the frontier between polar intermetallics and Zintl phases for the examples of the prolific ALnTnTe3-type alkali metal (A) lanthanide (Ln) late transition metal (Tn) tellurides. **2021**,	1
704	Synthesis, crystal and electronic structure of BaLi2Cd2Ge2. **2021**,	0

703	Realization of interstitial boron ordering and optimal near-surface electronic structure in Pd-B alloy electrocatalysts. **2021**, 419, 129568	10
702	Ultrafast crystallization mechanism of amorphous Ge15Sb85 unraveled by pressure-driven simulations. **2021**, 216, 117123	2
701	Revealing the mechanism of grain refinement and anti Si-poisoning induced by (Nb, Ti)B2 with a sandwich-like structure. **2021**, 219, 117265	1
700	New intermetallics R1+xZr1−xNi (R = Er–Tm, x ~ 0.5) with the TiNiSi type of structure. **2021**, 137, 107279	
699	Superhard carbon-rich C–N compounds hidden in compression of the mixture of carbon black and tetracyanoethylene. **2021**, 184, 846-854	0
698	Synthetic accessibility and stability rules of NASICONs. **2021**, 12, 5752	7
697	Crystal and electronic structures of the new ternary silicide Sc12Co41.8Si30.2. **2021**, 302, 122373	
696	Adsorption characteristics of silver atoms and silver ions on silica surface in silver nanoparticle hydrosol system. **2021**, 562, 150168	3
695	Transition metal single atom anchored C3N for highly efficient formic acid dehydrogenation: A DFT study. **2021**, 562, 150186	1
694	First-principles study on the P-induced embrittlement and de-embrittling effect of B and C in ferritic steels. **2021**, 219, 117260	3
693	Controlling Diphenyl Ether Hydrogenolysis Selectivity by Tuning the Pt Support and H-Donors under Mild Conditions. 12661-12672	0
692	Unraveling surface functionalization of Cr2B2T2 (T´=´OH, O, Cl, H) MBene by first-principles calculations. **2021**, 199, 110810	0
691	Boron doped Ni-rich LiNi0.85Co0.10Mn0.05O2 cathode materials studied by structural analysis, solid state NMR, computational modeling, and electrochemical performance. **2021**, 42, 594-607	2
690	Crystal structure, magnetic properties and bonding analysis of M3Pt23Ge11 (M=Ca, Sr, Ba and Eu). **2021**, 303, 122486	
689	Design of (C3N2H5)(1-x)CsxPbI3 as a novel hybrid perovskite with strong stability and excellent photoelectric performance: A theoretical prediction. **2021**, 233, 111401	3
688	Adsorption behaviors of NH3 and HCl molecules on Fe-based crystal planes: A DFT study. **2021**, 246, 116976	3
687	Temperature-dependent elastic and plastic properties of α2-Ti3Al. **2021**, 139, 107368	1
686	Hydrogen storage properties of hexagonal C14 Laves phase Cu2Cd: A DFT study. **2021**, 304, 122560	1

685	The role of S and Mo doping on the dissociation of water molecule on FeOCl surface: Experimental and theoretical analysis. **2021**, 426, 131353	4
684	Sulfur-doping promoting peroxone reaction over TiO2 for highly effective NO oxidation at low temperature: Experimental and DFT studies. **2022**, 429, 132475	2
683	Correlating structure and orbital occupation with the stability and mechanical properties of 3d transition metal carbides. **2022**, 891, 161866	3
682	Hidden spontaneous polarisation in the chalcohalide photovoltaic absorber SnSbSI. **2021**, 8, 2709-2716	8
681	Sr-doped SmMnO3 perovskites for high-performance near-isothermal solar thermochemical CO2-to-fuel conversion. **2021**, 5, 4295-4310	3
680	Localized vibration and avoided crossing in SrTi11O20 for oxide thermoelectrics with intrinsically low thermal conductivity. **2021**, 9, 11674-11682	1
679	Assessing Nickel Titanium Binary Systems Using Structural Search Methods and Ab Initio Calculations. **2021**, 125, 1578-1591	1
678	Materials Screening for Disorder-Controlled Chalcogenide Crystals for Phase-Change Memory Applications. **2021**, 33, e2006221	13
677	High-throughput computational search for high carrier lifetime, defect-tolerant solar absorbers. **2021**, 14, 5057-5073	6
676	M2As2Q5 (M = Ba, Pb; Q = S, Se): a source of infrared nonlinear optical materials with excellent overall performance activated by multiple discrete arsenate anions. **2021**, 9, 1156-1163	18
675	Conduction Band Control of Oxyhalides with a Triple-Fluorite Layer for Visible Light Photocatalysis. **2021**, 143, 2491-2499	20
674	The variation of intrinsic defects in XTe (X = Ge, Sn, and Pb) induced by the energy positions of valence band maxima. **2021**, 9, 5765-5770	5
673	Alloy engineering in mixed Sn□Ge perovskites for photovoltaic application. **2021**, 9, 6955-6961	4
672	Effect of Halogen Ions on the Low Thermal Conductivity of Cesium Halide Perovskite. **2021**, 125, 91-97	5
671	First principles and machine learning based superior catalytic activities and selectivities for N2 reduction in MBenes, defective 2D materials and 2D □-conjugated polymer-supported single atom catalysts. **2021**, 9, 9203-9213	9
670	Ab Initio Local-Energy and Local-Stress Calculations for Materials Science and Engineering. **2021**, 62, 1-15	5
669	Ferroelastic-switching-driven large shear strain and piezoelectricity in a hybrid ferroelectric. **2021**, 20, 612-617	28
668	Realization of the Zn oxidation state. **2021**, 13, 14041-14048	1

667	Bonding diversity in rock salt-type tellurides: examining the interdependence between chemical bonding and materials properties.. **2021**, 11, 20679-20686	4
666	Difference in magnetic anisotropy of the ferromagnetic monolayers VI3 and CrI3. **2021**, 103,	9
665	High-throughput computational discovery of ternary-layered MAX phases and prediction of their exfoliation for formation of 2D MXenes. **2021**, 13, 7294-7307	15
664	Eine NiAs-artige Hochdruckmodifikation von FeN. **2017**, 129, 7408-7412	2
663	Itinerant Ferromagnetism and Antiferromagnetism from a Chemical Bonding Perspective. **2002**, 433-444	12
662	Theoretical Studies of Electronic Properties of Conjugated Polymers. **2001**, 39-87	5
661	Beyond-carbon-solvency effects of catalytic metal Ni on diamond growth. **2020**, 107, 107875	3
660	Molecular reactions and oxidation corrosion on UN (001) surface under exposure to environment gases: A DFT study. **2020**, 533, 152095	2
659	Crystal Structures, Superconducting Properties, and the Coloring Problem in ReAlSi and ReGaSi. **2020**, 59, 17310-17319	2
658	Shallow Valence Band of Rutile GeO2 and P-type Doping. **2020**, 124, 25721-25728	6
657	Sulfurized Polyacrylonitrile for High-Performance Lithium-Sulfur Batteries: In-Depth Computational Approach Revealing Multiple Sulfur's Reduction Pathways and Hidden Li Storage Mechanisms for Extra Discharge Capacity. **2021**, 13, 491-502	10
656	Chapter 5:Chemical Bonding Investigations for Materials. **2018**, 117-175	2
655	Tensorial elastic properties and stability of interface states associated with Σ(210) grain boundaries in Ni(Al,Si). **2017**, 18, 273-282	13
654	Charge-induced high-performance actuation of borophene. **2021**, 54, 105504	4
653	Electronic origin of grain boundary segregation of Al, Si, P, and S in bcc-Fe: combined analysis of ab initio local energy and crystal orbital Hamilton population. **2021**, 29, 015001	5
652	Topological phase transition from T-carbon to bct-C16. **2020**, 22, 073036	4
651	Pressure-induced decomposition of binary lanthanum intermetallic compounds. **2020**, 101,	4
650	Antiferromagnetic ground state in the MnGa4 intermetallic compound. **2018**, 2,	7

649	Intrinsic point defects and intergrowths in layered bismuth triiodide. **2018**, 2,	7
648	Polar metallic behavior of strained antiperovskites ACNi3(A=Mg,Zn,and Cd) from first principles. **2018**, 2,	10
647	High-throughput design of 211 M2AX compounds. **2019**, 3,	6
646	High thermoelectric performance in BaAgYTe3 via low lattice thermal conductivity induced by bonding heterogeneity. **2019**, 3,	15
645	Measurement of f orbital hybridization in rare earths through electric dipole-octupole interference in x-ray absorption spectroscopy. **2019**, 3,	4
644	Insights into the elastic properties of RE-i-MAX phases and their potential exfoliation into two-dimensional RE-i-MXenes. **2020**, 4,	11
643	Possible high-potential ilmenite type Na1MO3 (M=V Ni) cathodes realized by dominant oxygen redox reaction. **2020**, 4,	1
642	Atomic locations of minor dopants and their roles in the stabilization of Cu6Sn5. **2020**, 4,	3
641	Antiferroelectricity and robust dielectric response owing to competing polar and antipolar instabilities in tetragonal tungsten bronze K2RNb5O15 (R: rare-earth). **2020**, 4,	2
640	Chemical bonding in metallic glasses from machine learning and crystal orbital Hamilton population. **2020**, 4,	0
639	Ternary hypervalent silicon hydrides via lithium at high pressure. **2020**, 4,	3
638	Interplay between breathing and polar instabilities in transition metal perovskites with active A-sites. **2020**, 2,	1
637	The many flavours of halogen bonds - message from experimental electron density and Raman spectroscopy. **2019**, 75, 1190-1201	5
636	Bonding network and stability of clusters: the case study of AlTM pseudo-tenfold surfaces. **2019**, 75, 314-324	16
635	Site-Preference among Three Anions in the Quaternary BaAl4-Type Structure: Experimental and Computational Investigations for BaLi1.09(1)In0.91Ge2. **2013**, 34, 3847-3850	8
634	Lithium Containing Rare-Earth Metal Germanide, Er3.93Li1.07Ge4: Synthesis, Crystal Structure and Chemical bonding. **2013**, 34, 1579-1582	3
633	Structural Characterization of the Intermetallic Phase EuZnxIn4-x(x 1.1-1.2). Zn and In Site-Preferences in the BaAl4Structure-Type from Computational Analysis. **2013**, 34, 1656-1662	8
632	The role of halogen bonding in metal free phosphors. **2021**, 23, 23351-23359	

631	Stabilizing orthorhombic CsSnI3 perovskites with optimized electronic properties by surface ligands with inter-molecular hydrogen bond.	1
630	Theoretical insights into volatile iodine adsorption onto COF-DL229. **2021**, 23, 25365-25373	1
629	Construction of frustrated Lewis pairs on carbon nitride nanosheets for catalytic hydrogenation of acetylene. **2021**, 23, 24349-24356	3
628	Rational design of boron-containing co-doped graphene as highly efficient electro-catalysts for the nitrogen reduction reaction. **2021**, 9, 24590-24599	0
627	Stability and structural properties of vacancy-ordered and -disordered ZrCx. **2021**, 11, 32573-32589	1
626	Predictions of attainable compositions of layered quaternary -MAB phases and solid solution MAB phases. **2021**, 13, 18311-18321	0
625	Theoretical Prediction and Thin-Film Growth of the Defect-Tolerant Nitride Semiconductor YZn3N3.	2
624	Activating Lattice Oxygen in Perovskite Oxide by B-Site Cation Doping for Modulated Stability and Activity at Elevated Temperatures. **2021**, 8, e2102713	8
623	The modifications are highlighted in yellow. First principles study on the geometric and electronic properties of two-dimensional Nb2CT x Mxenes.	1
622	Identifying and Passivating Killer Defects in Pb-Free Double CsAgBiBr Perovskite. **2021**, 12, 10581-10588	3
621	Advances in Low-Frequency Vibrational Spectroscopy and Applications in Crystal Engineering.	3
620	Heteroanionic Ruddlesden-Popper ferroelectrics from anion order and octahedral tilts. **2021**, 5,	
619	Rb3Er4Cu5Te10: Exploring the Frontier between Polar Intermetallics and Zintl-Phases via Experimental and Quantumchemical Approaches.	1
618	Importance of Interfacial Structures in the Catalytic Effect of Transition Metals on Diamond Growth. **2021**, 6, 28432-28440	
617	Proposed Superconducting Electride Li_{6}C by sp-Hybridized Cage States at Moderate Pressures. **2021**, 127, 157002	1
616	Theoretical investigations of hydrogen absorption in the A15 intermetallics Ti3Sb and Ti3Ir. **2021**,	
615	Flux synthesis, crystal structure and electronic properties of the layered rare earth metal boride silicide Er3Si5□ B. An example of a boron/silicon-ordered structure derived from the AlB2 structure type. **2021**,	
614	Understanding the efficacy of concentrated interstitial carbon in enhancing the pitting corrosion resistance of stainless steel. **2021**, 221, 117433	8

613	Boron adsorption and its effect on stability and CO activation of Fe5C2 catalyst: An ab initio DFT study. **2021**, 627, 118382	0
612	Prediction of high-Tc superconductivity in ternary lanthanum borohydrides. **2021**, 104,	13
611	Origin of pure and C doped borophene stability and its activity for OER. **2022**, 574, 151613	3
610	Ga-doped Pd/CeO2 model catalysts for CO oxidation reactivity: A density functional theory study. **2021**, 151655	2
609	Capturing polysulfides by sulfurized-polyacrylonitrile in lithium-sulfur batteries and the sulfur-chain effects through Density Functional Theory.	1
608	Tuning Site Energy by XO Units in LiX(PO) Enables High Li Ion Conductivity and Improved Stability. **2021**, 13, 50948-50956	1
607	Theoretical Insights into Dual-Metal-Site Catalysts for the Nonoxidative Coupling of Methane. 13149-13159	3
606	Local perturbations of periodic systems. Chemisorption and point defects by GoGreenGo. **2021**, 42, 2352-2368	
605	Stabilizing indium sulfide for CO electroreduction to formate at high rate by zinc incorporation. **2021**, 12, 5835	19
604	Engineering of Ferroic Orders in Thin Films by Anionic Substitution. 2107135	4
603	Theoretical Design of Inorganic Flexible Bulk Photovoltaic Materials. **2021**, 12, 10182-10189	0
602	Theoretical Study of Anisotropic Carrier Mobility for Two-Dimensional NbSe Material. **2021**, 6, 26782-26790	1
601	Emerging Yttrium Phosphides with Tetrahedron Phosphorus and Superconductivity under High Pressures. **2021**, 27, 17420-17427	0
600	Chemical Bonding of Solids. **2010**, 111-131	
599	Novel compounds in the hafnium nitride system: first principle study of their crystal structures and mechanical properties. **2016**, 65, 118102	2
598	Growth, Structural and Electronic Properties of Functional Semiconductors Studied by First Principles. **2016**, 145-162	
597	iFeMnSiO (0.0, 0.5, 1.0; y = 0.0, 2.0) . **2018**, 550-559	
596	Anchoring effect of distorted octahedra on the stability and strength of platinum metal pernitrides. **2019**, 3,	1

595	Developments of Interorbital Band Interaction Analysis and Embedded Cluster Model Incorporating Periodic Electrostatic Potential for Supported Metal Catalysts. **2019**, 18, 49-63	
594	Vacancy-Ordered Double Perovskites. **2020**, 87-106	
593	New ternary MgCo2Ga5 and MgNi2Ga5 gallides. **2020**, 235, 513-521	0
592	First-principles investigation of two-dimensional 1T TiO2. **2020**, 4,	2
591	Toward Zero-Strain Mixed Conductors: Anomalously Low Redox Coefficients of Chemical Expansion in Praseodymium-Oxide Perovskites.	2
590	DFT-Guided Crystal Structure Redetermination and Lattice Dynamics of the Intermetallic Actinoid Compound UIr. **2021**, 60, 16686-16699	
589	Function of Doping Ru Element in the Hydrogen Evolution Reaction in Rare-Earth Transition-Metal Intermetallics. **2021**, 60, 16754-16760	0
588	Magnetostructural coupling from competing magnetic and chemical bonding effects. **2020**, 2,	
587	The synthesis mechanism of nitrogen to ammonia on the Fe, Co, Ni-doped Cu(1 0 0) Surface: A DFT study. **2022**, 573, 151477	0
586	Theoretical insights into mechanisms of electrochemical reduction of CO2 to ethylene catalyzed by Pd3Au. **2022**, 572, 151474	1
585	Coverage-dependent adsorption and stability of functionalized Ge(1 0 0) and (1 1 1) surfaces. **2022**, 572, 151466	
584	Local ordering and interatomic bonding in magnetostrictive Fe0.85Ga0.15X (X=Ni,Cu,Co,La) alloy. **2022**, 202, 110934	0
583	Bismuth Chalcoiodides. **2020**, 117-138	
582	Theoretical Methods. **2020**, 27-46	
581	Computational Methodology. **2020**, 35-49	
580	Prediction of short range order in high-entropy alloys and its effect on the electronic, magnetic and mechanical properties. **2020**, 69, 046102	2
579	Pd-P antibonding interactions in APd2P2 (A=Ca and Sr) superconductors. **2020**, 4,	1
578	Compression-induced resistance of singlet oxygen dissociation on phosphorene. **2020**, 4,	

577	Ab Initio Investigation on the Doped H3S by V, VI, and VII Group Elements Under High Pressure. 1	1
576	Computational Understanding of Fe-Pt Synergy in Promoting Guaiacol Hydrodeoxygenation. **2021**, 121985	0
575	Anionic Redox Regulated via Metal-Ligand Combinations in Layered Sulfides. **2021**, e2107353	1
574	Understanding the Oxygen-Vacancy-Related Catalytic Cycle for H2 Oxidation on Ceria-Based SOFC Anode and the Promotion Effect of Lanthanide Doping from Theoretical Perspectives. **2021**, 151803	3
573	Boron Coordination Effect in Ni-N Doped Graphene Catalysts on the ORR Performance Based on DFT Calculations. **2021**,	1
572	Computational Design of Pd Nanoclusters and Pd Single-Atom Catalysts Supported on O-Functionalized Graphene.	3
571	Theoretical Study of Weakly Bound Adsorbates on Au(111): Tests on van der Waals Density Functionals.	0
570	Comparative Study of Internal Mechanical Stresses in the Structures of Montmorillonite and Halloysite. **2020**, 46, 598-604	0
569	Rapid screening alloying elements for improved corrosion resistance on the Mg(0001) surface using first principles calculations. **2021**, 23, 26887-26901	3
568	Degradation intermediates of Amitriptyline and fundamental importance of transition metal elements in LDH-based catalysts in Heterogeneous Electro-Fenton system. **2022**, 283, 120225	1
567	Unveiling the Selectivity of CO2 Reduction on Cu2ZnSnS4: The Effect of Exposed Termination. **2021** , 125, 24967-24973	3
566	Comparable catalytic activity of a low-cost catalyst IrO2/TiO2 for methane conversion □A density functional theory study. **2021**, 151938	4
565	Metallic versus covalent interactions in Li-doped gallium clusters. **2021**, 23, 1	
564	Electronic Origin of Non-Zone-Center Phonon Condensation: Octahedral Rotation as a Case Study. **2021**, 127, 215701	2
563	Designing stable 2D materials solely from VIA elements. **2021**, 119, 223101	0
562	Activating Inert MXenes for Hydrogen Evolution Reaction via Anchored Metal Centers. 2100383	
561	A durable and pH-universal self-standing MoC-MoC heterojunction electrode for efficient hydrogen evolution reaction. **2021**, 12, 6776	26
560	Theoretical Study of the Propene Combustion Catalysis of Chromite Spinels: Reaction Mechanism and Relation between the Activity and Electronic Structure of Spinels. **2021**, 125, 25983-26002	0

559	Grain boundary kinetics in magnesium alloys from first principles. **2021**, 111042	1
558	Improved Hydrothermal Durability of Cu-SSZ-13 NH3-SCR Catalyst by Surface Al Modification: Affinity and Passivation. **2021**, 405, 199-199	3
557	Recent Studies on the Nature and State of Carbon Atoms in Iron. **2021**, 61, 2677-2686	
556	Theoretical insights to elastic and thermal properties of WB4 tetraborides: A first-principles calculation. **2021**, 110731	2
555	Investigation of Electronic Structure and Electrochemical Properties of Na2MnSiO4 as a Cathode Material for Na Ion Batteries. **2021**, 125, 25968-25982	1
554	First-principles investigation of uranium mononitride (UN): Effect of magnetic ordering, spin-orbit interactions and exchange correlation functional. **2021**, 153401	4
553	Adsorption based on weak interaction between phenolic hydroxyl, carboxyl groups and silver nanoparticles in aqueous environment: Experimental and DFT-D3 exploration. **2021**, 9, 106816	1
552	Mind the Mines: Lapieite Minerals with Ultralow Lattice Thermal Conductivity and High Power Factor for Thermoelectricity.	2
551	Synthesis and Transport Properties of the Family of Zintl Phases Ca3RESb3 (RE = La, Nd, Sm, Gd, Tm, Lu): Exploring the Roles of Crystallographic Disorder and Core 4f Electrons for Enhancing Thermoelectric Performance.	1
550	The Role of Zr in Co-Segregation Behavior of Zr- X Solutes and Their Effects on the Thermodynamic Stability and Fracture Strength of Ni Σ5 [001](210) Grain Boundary.	
549	Single-atom catalysts on supported silicomolybdic acid for CO2 electroreduction: a DFT prediction.	4
548	Two-dimensional InSb/GaAs- and InSb/InP-based tandem photovoltaic device with matched bandgap.. **2022**,	2
547	First examples of nickel–aluminum mixed chalcogenides based on the AuCu3-type fragments: Breaking a robust intermetallic bond system in Ni3Al. **2022**, 306, 122815	
546	Al coverage of AlN(0001) surface and Al vapor pressure – Thermodynamic assessment based on ab initio calculations. **2022**, 203, 111159	
545	Boundary in electrocatalytic hydrogen evolution reaction: From single metal to binary intermetallic compounds. **2022**, 162, 106378	1
544	Revealing the key role of bonding states in surface chemisorption. **2022**, 249, 117345	0
543	Interfacial electronic modulation on heterostructured NiSe@CoFe LDH nanoarrays for enhancing oxygen evolution reaction and water splitting by facilitating the deprotonation of OH to O. **2022**, 431, 134080	15
542	Single transition metal atom anchored on VSe2 as electrocatalyst for nitrogen reduction reaction. **2022**, 580, 152272	2

541	Effectively boosting selective ammonia synthesis on electron-deficient surface of MoB2. **2022**, 305, 121023	5
540	Roles of optical phonons and logarithmic profile of electron-phonon coupling integration in superconducting Sc0.5Y0.5H6 superhydride under pressures. **2022**, 901, 163524	2
539	Coordination-tuned Fe single-atom catalyst for efficient CO2 electroreduction: The power of B atom. **2022**, 433, 134270	2
538	Phase-dependent catalytic performance of MnO2 for solvent-free oxidation of ethybenzene with molecular oxygen. **2022**, 305, 121050	3
537	Unexpected band gap evolution and high carrier mobility sparked by the orbital variation in two-dimensional GaGeX (X = S, Se, Te). **2022**, 138, 115112	0
536	Atomic structures of twin boundaries in CoO. **2021**, 23, 25590-25596	1
535	Computational screening of single-atom alloys TM@Ru(0001) for enhanced electrochemical nitrogen reduction reaction.	6
534	The effect of oxygen impurities on the stability and structural properties of vacancy-ordered and -disordered ZrC .. **2022**, 12, 3198-3215	0
533	Comprehending the stability of Sr2+ immobilization in chemically bonded phosphate ceramic system: A mechanism study. **2022**,	
532	First-Principles Plane-Wave-Based Exploration of Cathode and Anode Materials for Li- and Na-Ion Batteries Involving Complex Nitrogen-Based Anions. **2022**, 34, 652-668	2
531	Pressure-stabilized hexafluorides of first-row transition metals.. **2022**,	1
530	Pressure-stabilized high-energy-density material YN.. **2022**, 34,	
529	Forming Platinide Phases under Pressure in the CsPt System. **2022**, 126, 2062-2069	
528	Optical Control of Multistage Phase Transition via Phonon Coupling in MoTe_{2}.. **2022**, 128, 015702	2
527	Synergistic Effect of Coordination Fields and Hydrosolvents on the Single-Atom Catalytic Property in H2O2 Synthesis: A Density Functional Theory Study. **2022**, 126, 2349-2364	6
526	Controlling interlayer magnetic coupling in the two-dimensional magnet Fe3GeTe2. **2022**, 105,	3
525	Atomical Reconstruction and Cationic Reordering for Nickel-Rich Layered Cathodes. 2103757	9
524	Enhanced covalency and nanostructured-phonon scattering lead to high thermoelectric performance in n-type PbS. **2022**, 24, 100953	2

523	Design Rules of a Sulfur Redox Electrocatalyst for Lithium-sulfur Batteries.. **2022**, e2110279	16
522	Pressure-induced evolution of crystal and electronic structure of neptunium hydrides.. **2022**,	
521	Sn 7 Br 10 S 2 : The First Ternary Halogen-Rich Chalcohalide Exhibiting a Chiral Structure and Pronounced Nonlinear Optical Properties.	0
520	Lowering the C□H bond activation barrier of methane by means of SAC@Cu(111): periodic DFT investigations. **2021**, 46, 70-74	2
519	Partitioning of noble gases (He, Ne, Ar, Kr, Xe) during Earth□s core segregation: A possible core reservoir for primordial noble gases. **2022**, 321, 329-329	2
518	Controlling the nucleation and growth of ultrasmall metal nanoclusters with MoS grain boundaries.. **2022**,	0
517	Penta-CN2 revisited: Superior stability, synthesis condition exploration, negative Poisson□s ratio and quasi-flat bands. **2022**, 585, 152536	1
516	Electronic and optical properties of hydrogen-terminated biphenylene nanoribbons: a first-principles study. **2021**,	3
515	A superconducting boron allotrope featuring anticlinal pentapyramids. **2022**, 10, 672-679	1
514	Discovery of Electrides in Electron-Rich Non-Electride Materials via Energy Modification of Interstitial Electrons. 2112198	1
513	Designing Conductive-Bridge Phase-Change Memory to Enable Ultralow Programming Power.. **2022**, e2103478	8
512	Effects of potassium on propylene epoxidation by molecular oxygen on Cu2O (111): a DFT study.	0
511	Formation of twelve-fold iodine coordination at high pressure.. **2022**, 13, 412	4
510	Establishing the Principal Descriptor for Electrochemical Urea Production via the Dispersed Dual-Metals Anchored on the N-Decorated Graphene.. **2022**, e2105697	2
509	Sn7Br10S2: The First Ternary Halogen-Rich Chalcohalide Exhibiting A Chiral Structure and Pronounced Nonlinear Optical Properties.. **2021**,	7
508	TMN4 complex embedded graphene as efficient and selective electrocatalysts for chlorine evolution reactions. **2022**, 907, 116071	4
507	High electrocatalytical performance of FeCoNiCuPd high-entropy alloy for nitrogen reduction reaction. **2022**, 519, 112141	1
506	First-Principles Study of Transition Metal Ti-Based MXenes (Ti2MC2Tx and M2TiC2Tx) as Anode Materials for Sodium-Ion Batteries.	1

505	Modulating Crystal and Interfacial Properties by W-Gradient Doping for Highly Stable and Long Life Li-Rich Layered Cathodes. 2113013	7
504	Bridge the activity and durability of Ruthenium for hydrogen evolution reaction with the RuOC link. **2022**, 433, 134421	4
503	Semiconducting Sm3GaSe5O with trigonal bipyramidal GaSe5 units. **2022**, 308, 122901	0
502	Annihilation dynamics of a dislocation pair in graphene: Density-functional tight-binding molecular dynamics simulations and first principles study. **2022**, 205, 111224	1
501	Origin of the concentration-dependent effects of N on the stability and electrical resistivity in polycrystalline Ge1Sb2Te4.	0
500	Chemical-Mechanical Effects in Ni-Rich Cathode Materials.	3
499	Be[B2(SO4)4] □A Borosulfate exhibiting Ino- and Phyllosilicate Analogue Topology.	0
498	Investigation of out-of-plane ordered TiMoSiBfrom first principles.. **2022**,	0
497	Semiconducting and Metallic Compounds within the IrIn Structure Type: Stability and Chemical Bonding.. **2022**,	0
496	Thiotetrelates LiZnXS (X = Si, Ge, and Sn) As Potential Li-Ion Solid-State Electrolytes.. **2022**,	0
495	The Importance of Avoided Crossings in Understanding High Valley Degeneracy in Half-Heusler Thermoelectric Semiconductors. 2101367	3
494	Electrochemical CO2 Reduction On Two-Dimensional Metal 1,3,5-triamino-2,4,6- Benzenetriol Frameworks: A Density Functional Study.	0
493	Ammonia Synthesis on the RRuSi(001) (R = Ca,La) Surfaces: DFT Insights Revealing the Active La Termination of the LaRuSi Electride.	0
492	A multi-scale model for syngas combustion on NiO oxygen carrier for chemical looping combustion: The role of nearest neighbors. **2022**, 229, 107172	2
491	3.4% Solar-to-Ammonia Efficiency from Nitrate Using Fe Single Atomic Catalyst Supported on MoS 2 Nanosheets. 2108316	14
490	Optimally Selecting Photo- and Electrocatalysis to Facilitate CH Activation on TiO(110) Surface: Localized Photoexcitation versus Global Electric-Field Polarization.. **2022**, 2, 188-196	3
489	Lone pair driven anisotropy in antimony chalcogenide semiconductors.. **2022**,	3
488	Theoretical Insight on Why N-Vacancy Promotes the Selective Co2 Reduction to Ethanol on Nimn Doped Graphitic Carbon Nitride Sheets.	

487	Oxalate promoted iron dissolution of hematite via proton coupled electron transfer.	0
486	Trend in light-induced excited-state spin trapping in Fe(II)-based spin crossover systems.. **2022**,	1
485	Origin of the enhanced edge optical transition in transition metal dichalcogenide flakes. **2022**, 10, 5303-5310	
484	Anisotropic electrene T'-CaP with electron gas magnetic coupling as anode material for Na/K ion batteries.. **2022**,	0
483	Finite-momentum excitons and the role of electron-phonon couplings in the electronic and phonon transport properties of boron arsenide.. **2022**,	0
482	Zinc Germanium Nitrides and Oxide Nitrides: The Influence of Oxygen on Electronic and Structural Properties..	
481	Regulating Anionic Redox Activity of Lithium-Rich Layered Oxides Via Linbo3 Integrated Modification.	
480	Bonding dependent lithium storage behavior of molybdenum oxides for next-generation Li-ion batteries. **2022**, 10, 7718-7727	1
479	Materials design, synthesis, and transport properties of disordered rare-earth Zintl bismuthides with the -ThP structure type.. **2022**,	0
478	Hydrogen Storage Properties of Ternary Ordered Cubic Laves Phase Cu3cd2in: Electronic Structure and Bonding Approach.	
477	Structural Diversity and Unusual Valence States in Compressed Na-Hg System.	
476	Engineering Lattice Disorder on a Photocatalyst: Photochromic BiOBr Nanosheets Enhance Activation of Aromatic C-H Bonds via Water Oxidation.. **2022**,	11
475	Boron bridged NiN4B2Cx single-atom catalyst for superior electrochemical CO2 reduction. **2022**,	1
474	Evolution of Bonding and Magnetism Changes in Valence Electron Count in CuFeCoGe.. **2022**,	
473	Microscopic Mechanism of the Heat-Induced Blueshift in Phosphors and A Logarithmic Energy Dependence on the Nearest Dopant-Vacancy Distance.. **2022**,	4
472	Synthesis of cobalt single atom catalyst by a solid-state transformation strategy for direct C-C cross-coupling of primary and secondary alcohols. 1	2
471	Unusual phase transitions in two-dimensional telluride heterostructures. **2022**,	1
470	First-principles study of oxygen vacancy formation in strained oxides. **2022**, 131, 075106	1

469	Metal-Coordinating Single-Boron Sites Confined in Antiperovskite Borides for N2-to-NH3 Catalytic Conversion. **2022**, 12, 2967-2978	1
468	Electronic Structures of Group III–V Element Haeckelite Compounds: A Novel Family of Semiconductors, Dirac Semimetals, and Topological Insulators. 2110930	0
467	LModeA-nano: A PyMOL Plugin for Calculating Bond Strength in Solids, Surfaces, and Molecules via Local Vibrational Mode Analysis.. **2022**, 18, 1821-1837	0
466	Graph-based discovery and analysis of atomic-scale one-dimensional materials.	1
465	From simple to complex crystal chemistry in the RE–Au–Tt systems (RE = La, Ce, Pr, Nd; Tt = Ge, Pb).	0
464	Microscopic Mechanism of the Heat-Induced Blueshift in Phosphors and a Logarithmic Energy Dependence on the Nearest Dopant–Vacancy Distance. **2022**, 134,	
463	Substantial Improvement of Operating Stability by Strengthening Metal-Halogen Bonds in Halide Perovskites. 2112129	2
462	Pressure-tuned one- to quasi-two-dimensional structural phase transition and superconductivity in LiP15. **2022**, 105,	
461	Vacancy ordering in substoichiometric zirconium carbide: A review.	0
460	Arsenene Monolayer: A Promising Electrocatalyst for Anodic Chlorine Evolution Reaction. **2022**, 12, 296	0
459	Influence of local structural distortion on the magnetism of Na2IrO3 compounds. **2022**, 105,	1
458	Electronic Effect or Underpotentially Deposited Hydrogen? Insights into the effect of Pb on formic acid electro-oxidation on Pt.	0
457	Orthorhombic ScB3 and hexagonal ScB6 with high hardness. **2022**, 105,	0
456	Hypervalency in amorphous chalcogenides.. **2022**, 13, 1458	0
455	SrAl5Pt3 and Sr2Al16Pt9 – two new strontium aluminum platinides. **2022**,	1
454	Predicting the stability and electronic structure of alkali metal aurides.. **2022**,	
453	Two-Dimensional Palladium Phosphoronitride for Oxygen Reduction.. **2022**,	1
452	Uncovering the Mechanism of the Hydrogen Poisoning on Ru Nanoparticles via Density Functional Theory Calculations. **2022**, 12, 331	2

451	Single Atoms Anchored in Hexagonal Boron Nitride for Propane Dehydrogenation from First Principles.	2
450	Multiferroicity and giant in-plane negative Poisson□ ratio in wurtzite monolayers. **2022**, 8,	0
449	Degenerated Hole Doping and Ultra-Low Lattice Thermal Conductivity in Polycrystalline SnSe by Nonequilibrium Isovalent Te Substitution.. **2022**, e2105958	1
448	Existence of BeCN and Its First-Principles Phase Diagram: Be and C Introducing Structural Diversity.. **2022**,	3
447	Structural and Theoretical Investigations on the Unique Coloring Scheme of the □Brass Type Phase: Cu 5+□Cd 8-□(□1.0□□0.1).	
446	Lattice dynamics and its effects on magnetocrystalline anisotropy energy of pristine and hole-doped YCo5 from first principles. **2022**, 105,	1
445	Interrelationship of bonding strength with structural stability of ternary oxide phases of MgSnO3: A first-principles study. **2022**, 413896	0
444	Tuning the size of skyrmion by strain at the Co/Pt interfaces.. **2022**, 25, 104039	1
443	Investigation on the solidification behavior in a brazed joint of the □strengthened Co-based single crystal superalloy. **2022**, 186, 111793	1
442	Adsorption Characteristics of Gas Molecules Adsorbed on Graphene Doped with Mn: A First Principle Study.. **2022**, 27,	1
441	Enhanced HER catalysis based on MXene/N-doped graphene heterostructures: A first-principles study. **2022**,	0
440	Design of Single-Atom and Frustrated-Lewis-Pair dual active sites for direct conversion of CH4 and CO2 to acetic acid. **2022**, 408, 206-215	4
439	New ternary phosphides RE5Pd9P7 (RE = Tm, Lu): synthesis, crystal and electronic structure.	
438	Revealing the impact of acceptor dopant type on the electrical conductivity of sodium bismuth titanate. **2022**, 229, 117808	0
437	Zirconium-enhanced segregation tendency of solutes X and Zr-X co-segregation induced synergistic/antagonistic effects on Ni □ [001](210) grain boundary. **2022**, 31, 103319	1
436	Effect of hybridization in PdAlY-(Ni/Au/Ir) metallic glasses thin films on electrical resistivity. **2022**, 214, 114681	
435	Interface bonding and failure mechanism of Ti(001)/Si(001) and TiO2(001)/Si(001) interfaces: A first□principles study. **2022**, 30, 101833	
434	Influencing mechanism of alkali metals on the adsorption property of NH3, NO, O2 and dehydrogenation reaction of NH3 on the □MnO2 (1 1 0) surface: A DFT´+´U study. **2022**, 318, 123470	1

433	Au decorated Pd nanowires for methane oxidation to liquid C1 products. **2022**, 308, 121223	0
432	Surface effect of the MgCl2 support in Ziegler Natta catalyst for ethylene polymerization: A computational study. **2022**, 589, 153002	9
431	Tandem catalysis on adjacent active motifs of copper grain boundary for efficient CO2 electroreduction toward C2 products. **2022**, 70, 219-223	4
430	Enhanced water splitting photocatalyst enabled by two-dimensional GaP/GaAs van der Waals heterostructure. **2022**, 591, 153198	2
429	Adsorption of NO2 and CO molecules on Ni (1 1 1) supported defective Graphene: A DFT study. **2022**, 590, 153027	0
428	Understanding the effect of transition metals and vacancy boron nitride catalysts on activity and selectivity for CO2 reduction reaction to valuable products: A DFT-D3 study. **2022**, 319, 123808	1
427	Strain tunable intrinsic ferromagnetic in 2D square CrBr2. **2021**, 11, 115220	1
426	A Low-Temperature Structural Transition in Canfieldite, AgSnS, Single Crystals. **2021**,	1
425	Ternary Mg-Nb-H polyhydrides under high pressure. **2021**, 104,	2
424	Improvement of Thermoelectric Properties via Texturation Using a Magnetic Slip Casting Process The Illustrative Case of CrSi2. **2022**, 34, 1143-1156	0
423	Local structure analysis of Sb, Bi, and Ag dopant atoms in Mg2Si semiconductor by x-ray absorption spectroscopy and first-principles calculation. **2021**, 130, 245105	0
422	Abnormally Low Lattice Thermal Conductivity in ABX Honeycomb Compounds. **2021**, 16,	3
421	Electronic properties of the topological kagome metals YV6Sn6 and GdV6Sn6. **2021**, 104,	2
420	Stabilizing a Nickel-Rich (LiNi0.89Co0.055Mn0.055O2) Cathode Material by Doping Zirconium or Molybdenum: A First-Principles Study. **2021**, 125, 27543-27555	4
419	Superconducting hydrogen tubes in hafnium hydrides at high pressure. **2021**, 104,	1
418	Experimental and Theoretical Study on the Substitution Patterns in Lithium Germanides: The Case of Li 15 Ge 4 vs Li 14 ZnGe 4. **2022**, 2022,	
417	Transition Metal and N Doping on AlP Monolayers for Bifunctional Oxygen Electrocatalysts: Density Functional Theory Study Assisted by Machine Learning Description.. **2021**,	5
416	Discovery of Lead-Free Perovskites for High-Performance Solar Cells via Machine Learning: Ultrabroadband Absorption, Low Radiative Combination, and Enhanced Thermal Conductivities.. **2021**, e2103648	8

415	Metavalent bonding in chalcogenides: DFT-chemical pressure approach.. **2022**,	1
414	Stable freestanding two-dimensional anionic electrons in YCl with extremely weak interlayer interaction.	0
413	Theoretical predictions of phase stability for orthorhombic and hexagonal ternary MAB phases.. **2022**,	0
412	Atomistic modeling of Li- and post-Li-ion batteries. **2022**, 6,	1
411	Bond formation at polycarbonate | X interfaces (X = Ti, Al, TiAl) probed by X-ray photoelectron spectroscopy and density functional theory molecular dynamics simulations. **2022**, 153363	
410	Activating lattice oxygen in NiFe-based (oxy)hydroxide for water electrolysis.. **2022**, 13, 2191	16
409	Prediction of Large Second Harmonic Generation in the Metal-Oxide/Organic Hybrid Compound CuMoO3(p2c). **2022**, 14, 824	
408	First-Principles Study of Honeycomb Borophene on the Mo2C Substrate.	0
407	Low-Dimensional Metal□Organic Frameworks with High Activity and Selectivity toward Electrocatalytic Chlorine Evolution Reactions.	2
406	Epitaxial ScxAl1□N on GaN exhibits attractive high-K dielectric properties. **2022**, 120, 152901	5
405	Electrochemistry of P-C Bonds in Phosphorus-Carbon Based Anode Materials.. **2022**,	1
404	Effect of Surface [Cu4O] Moieties on the Activity of Cu-Based Catalysts. 5162-5173	1
403	Impurity Combination Effect on Oxygen Absorption in □2-Ti3Al. **2022**, 12, 650	
402	Molecular insight into iron corrosion induced by chloride and sulphate. **2022**, 209, 111429	1
401	Dilute carbon in H3S under pressure. **2022**, 8,	2
400	Theoretical understanding of oxygen stability in Mn□e binary layered oxides for sodium-ion batteries.	
399	Transition metal decorated phthalocyanine as a potential host material for lithium polysulfides: a first-principles study.. **2022**, 12, 13975-13984	0
398	Unraveling the relationships between chemical bonding and thermoelectric properties: n-type ABO3 perovskites.	1

397	MgH2/Single-Atom Heterojunctions: Effective Hydrogen Storage Materials with Facile Dehydrogenation.	0
396	Electrocatalytic CO2 reduction reaction on dual-metal- and nitrogen-doped graphene: coordination environment effect of active sites.	2
395	Building up the Genome of bi-atom catalysts toward efficient HER/OER/ORR.	5
394	An extended computational approach for point-defect equilibria in semiconductor materials. **2022**, 8,	0
393	Insights Into the Electronic Properties of PbBi Atomic Layers on Ge(111) and Si(111) Surfaces. **2022**, 9,	0
392	Phase variation of ferroelectric Li2Sr1 Cax(Nb1 . **2022**, 6,	0
391	Effect of carbon atoms on the reliability of potassium-ion electrets used in vibration-powered generators.	1
390	Formation and stability of Rh2Cd5 and its strucural correlation with RhCd and Rh3Cd5 (~ 0.56). **2021**,	
389	Unraveling Electronic Trends in O* and OH* Surface Adsorption in the MO2 Transition-Metal Oxide Series. **2022**, 126, 7903-7909	0
388	Improved Thermoelectric Photovoltaic Performance of Ag2Se Originating from a Halogenation-Induced Wider Band Gap and Low Crystal Symmetry.	0
387	Materials under high pressure: a chemical perspective. **2022**, 128, 1	2
386	3D Analogs of Square-Net Nodal Line Semimetals: Band Topology of Cubic LaIn3.	1
385	Electronic Band Structure. **2022**, 41-93	
384	Pressure-induced stable structures and physical properties in Sr-Ge System.	
383	Reversible hydrogen storage for NLi4-Decorated honeycomb borophene oxide. **2022**,	1
382	Structure Property Relationship of Oxygen-Doped Two-Dimensional Gallium Selenide for Hydrogen Evolution Reaction Revealed from Density Functional Theory.	0
381	First-principles computational tensile test of Fe grain boundaries considering the effect of magnetism: Electronic origin of grain boundary embrittlement due to Zn segregation. **2022**, 6,	0
380	Hydrogen storage properties of ternary ordered cubic Laves phase Cu3Cd2In: Electronic structure and bonding approach. **2022**, 312, 123223	0

379	Nitriding behavior and mechanical properties of AerMet100 steel and first-principles calculations of phase interfaces. **2022**,	0
378	Potential of Intrinsic Reactivity toward Value Added Products from Methane Oxidation on RhO2(110) Surface. **2022**, 153499	1
377	Stabilizing single-atomic ruthenium by Ferrous ion doped NiFe-LDH towards highly efficient and sustained water oxidation. **2022**, 136962	0
376	Electronic structure of chabazite zeolites H-SSZ-13 and H-SAPO-34. **2022**, 338, 111957	0
375	Atomistic explanation of failure mechanisms of thermoelectric type-VIII clathrate Ba8Ga16Sn30. **2022**, 31, 103605	
374	Ag rearrangement induced metal-insulator phase transition in thermoelectric MgAgSb. **2022**, 25, 100702	
373	The effect of grain boundary in hexagonal boron nitride on catalytic activity of nitrogen reduction reaction. **2022**, 593, 153468	0
372	Theoretical insight on why N-vacancy promotes the selective CO2 reduction to ethanol on NiMn doped graphitic carbon nitride sheets. **2022**, 595, 153527	3
371	DensityTool: A post-processing tool for space- and spin-resolved density of states from VASP. **2022**, 277, 108384	2
370	Structural and mechanistic study of antimonite complexation with organic ligands at the goethite-water interface.. **2022**, 134682	0
369	Unraveling the mechanism of ligands regulating electronic structure of MN4 sites with optimized ORR catalytic performance. **2022**, 595, 153526	2
368	Structural diversity and hydrogen storage properties in the system K-Si-H.. **2022**,	
367	Origin of Bismuth-Rich Strategy in Bismuth Oxyhalide Photocatalysts.	2
366	Pressure-Driven Ne-Bearing Polynitrides with Ultrahigh Energy Density. **2022**, 39, 056102	0
365	Using in-plane anisotropy to engineer Janus monolayers of rhenium dichalcogenides. **2022**, 6,	
364	Optoelectronic and mechanical properties of the orthogonal and tetragonal Cu2CdGe(SxSe1−x)4 semiconducting system via first principles methods. **2022**, 131, 205701	1
363	Configuration stability and electronic properties of diamane with boron and nitrogen dopants. **2022**, 105,	
362	H2 Activation on Pristine and Substitutional ZnO(101 0) and Cr2O3(001) Surfaces by Density Functional Theory Calculations.	2

361	How arsenic makes amorphous GeSe a robust chalcogenide glass for advanced memory integration. **2022**, 218, 114834	1
360	Chemical Templates That Assemble the Metal Superhydrides.	0
359	Insights into Cation-Disorder Effect on Stability, Electronic Structure and Defect Properties of Zn-Iv-Nitrides: The Case of Zngen2.	
358	Crystal structure, electronic structure and phase stability of the Cu2-xMxCd (M=Zn, Ga, Ge, Sn) pseudo-binary Laves phases: Effect of valence electron concentration. **2022**, 123283	1
357	A theoretical framework for oxygen redox chemistry for sustainable batteries.	1
356	Al4Ir: An Al□r Binary-Phase Superstructure of the Ni2Al3 Type.	
355	Understanding the structure of Cu-doped MgAl2O4 for CO2 hydrogenation catalyst precursor using experimental and computational approaches. **2022**,	1
354	Quasi-Covalently Coupled Ni□u Atomic Pair for Synergistic Electroreduction of CO2.	8
353	Dimensionality switching and superconductivity transition in dense 1T□HfSe2. **2022**, 105,	0
352	The Key Role of Competition between Orbital and Electrostatic Interactions in the Adsorption on Transition Metal Single-Atom Catalysts Anchored by N-doped Graphene.	4
351	Insights into the influence of functional groups on the properties of graphene from first-principles calculations.	0
350	Direct d□ hybridization mechanism for strong anisotropic carrier transport in layered Mo2SBr2. **2022**, 105,	0
349	Excellent Thermoelectric Performance of the Metal Sulfide CuTaS3.	1
348	Stability, metallicity, and magnetism in niobium silicide nanofilms. **2022**, 6,	
347	Quantum spin Hall effect in two-dimensional transition-metal chalcogenides MX5 (M = Zr, Hf and X = S, Se, Te). **2022**, 143, 115325	0
346	Effect of defective structure taking on the electronic and optical properties of InP nanowire. **2022**, 640, 414042	
345	Insight into Electron Transport Performance of Fapbi3-Sno2 Interface: A First-Principles Study.	
344	Exploring the synergistic effect of alloying toward hydrogen evolution reaction: a case study of Ni3M (M = Ti, Ge and Sn) series.	

343	Computational understanding role of vacancies and distortions in wurtzite ferroelectric memory materials: implications for device miniaturization.	1
342	Temperature-dependence of the band gap in the all-inorganic perovskite CsPbI3 from room to high temperatures.	1
341	Theoretically identifying the electrocatalytic activity and mechanism of Zn doped 2D h-BN for nitrate reduction to NH3. **2022**, 58, 7156-7159	1
340	Giant bulk photovoltaic effect driven by the wall-to-wall charge shift in WS2 nanotubes. **2022**, 13,	1
339	How to Change the Reaction Chemistry on Non-Precious Metal Oxide Nanostructure Materials for Electrocatalytic Oxidation of Biomass-Derived Glycerol to Renewable Chemicals?. 2203285	1
338	Growth mechanism and self-polarization of bilayer InSb (111) on Bi (001) substrate. **2022**, 34, 335001	
337	Examination of a Structural Preference in Quaternary Alkali-Metal (A) Rare-Earth (R) Copper Tellurides by Combining Experimental and Quantum-chemical Means. **2022**, 61, 9269-9282	1
336	Uncovering the Nature of Band Gap Engineering of Adsorption Energy by Elucidating an Adsorbate Bonding Mechanism on Two-Dimensional TiO2(110).	
335	Activated chemical bonds in nanoporous and amorphous iridium oxides favor low overpotential for oxygen evolution reaction. **2022**, 13,	3
334	Cation-doped ZnS catalysts for polysulfide conversion in lithium–sulfur batteries. **2022**, 5, 555-563	13
333	Two-dimensional tetragonal and hexagonal lattices of transition metal carbides MC (M = Ti, Zr, Hf): Observation of two nodal loops and strong light-harvesting ability. **2022**, 120, 243101	0
332	Metal-Rich Phosphides Obtained from the Lead Flux: Synthesis, Crystal, and Electronic Structure of Sr5Pt12P9 and BaPt3P2. **2022**, 61, 9173-9183	1
331	Decoupled atomic contribution boosted high thermoelectric performance in mixed cation spinel oxides ACo2O4. **2022**, 120, 243901	1
330	Influence of Cu Doping on the Hydration of Dicalcium Silicate: A First-Principles Study. **2022**, 10, 8094-8104	1
329	Ab initio molecular dynamics simulation of structural and elastic properties of SiO 2 -P 2 O 5 -Al 2 O 3 -Na 2 O glass.	
328	Origin of supertetragonality in BaTiO3. **2022**, 6,	
327	Automated Bonding Analysis with Crystal Orbital Hamilton Populations.	1
326	Superconductivity in S-rich phases of lanthanum sulfide under high pressure. **2022**, 6,	0

325	Structural diversity and unusual valence states in compressed Na-Hg system. **2022**, 211, 111561	
324	Computational screening and catalytic origin of transition metal supported on g-t-C3N4 as single-atom catalysts for nitrogen reduction reaction. **2022**, 599, 153880	0
323	Oriented construction Cu3P and Ni2P heterojunction to boost overall water splitting. **2022**, 448, 137706	2
322	Electrocatalytic activity of □Sb two-dimensional surface for hydrogen evolution reaction.	1
321	The rise of MAX phase alloys - large-scale theoretical screening for prediction of chemical order and disorder.	2
320	Unveiling hybridization between the Cr-impurity-mediated flat band and the Rashba-split state of □-Au/Si(111) surface.	0
319	Insights into Cation-Disorder Effect on Stability, Electronic Structure and Defect Properties of Zn-Iv-Nitrides: The Case of Zngen2.	
318	Work Function Regulation of Surface-engineered Ti2CT2 MXene for Efficient Electrochemical Nitrogen Reduction Reaction.	0
317	Möbius-aromatic interlocked Mn2B10H10 wheel to metal-doped boranaphthalene M2@B10H8 and M2B5 2D-sheets (M = Mn and Fe): A Molecules to Materials continuum using DFT Study.	0
316	Insights into syngas to methanol conversion on Cr2O3 oxide from first-principles-based microkinetic simulations.	0
315	Al-Doping Driven Suppression of Capacity and Voltage Fadings in 4d-Element Containing Li-Ion-Battery Cathode Materials: Machine Learning and Density Functional Theory. 2201497	5
314	Effects of Ca2+ź-Mg2+ substitution on the properties of cementitious tobermorite. **2022**, 6,	
313	Insights Into to the KX (X = Cl, Br, I) Adsorption-Assisted Stabilization of CsPbI 2 Br Surface. 2202623	2
312	Electronic Modulation of Ru Nanosheet by d□ Orbital Coupling for Enhanced Hydrogen Oxidation Reaction in Alkaline Electrolytes. 2202404	1
311	Interplay between Oxygen Octahedral Rotation and Deformation in the Acentric ARTiO4 Series toward Negative Thermal Expansion.	1
310	Toward Complete Exfoliation of the Chemisorbed Two-Dimensional Iron Silicates on Ru(0001) via Hydrogenation.	0
309	First-principles indicators of ferroic parameters in epitaxial BiFeO3 and BiCrO3. **2022**, 132, 024102	
308	Identifying Substrate-Dependent Chemical Bonding Nature at Molecule/Metal Interfaces Using Vibrational Sum Frequency Generation Spectroscopy and Theoretical Calculations. **2022**, 126, 11298-11309	0

307	Photocatalytic Reduction of Carbon Dioxide to Methane at the Pd-Supported TiO2 Interface: Mechanistic Insights from Theoretical Studies. **2022**, 12, 8558-8571	1
306	Anionic Redox Chemistry for Sodium-Ion Batteries: Mechanisms, Advances, and Challenges.	1
305	Investigating the Structural Symmetrization of CsI3 at High Pressures through Combined X-ray Diffraction Experiments and Theoretical Analysis. **2022**, 61, 10977-10985	0
304	From molecular adsorption to decomposition of methanol on various ZnO facets: A periodic DFT study. **2022**, 154150	1
303	Self-assembled cobalt hydroxide micro flowers from nanopetals: Structural, fractal analysis and molecular docking study. **2022**, 32, 102163	0
302	Band engineering and improved thermoelectric performance in p-type SmMg2Sb2: A first-principles study. **2022**, 27, 100779	
301	Regulating anionic redox activity of lithium-rich layered oxides via LiNbO3 integrated modification. **2022**, 101, 107555	0
300	The metal-insulator transitions of VO 2 : A band theoretical approach. **2002**, 514, 650-704	41
299	Prediction of Core Electron Reactivity and High Oxidation States in Radium under High Pressure.	
298	Ferroelasticity in Two-Dimensional Tetragonal Materials. **2022**, 129,	3
297	First-principles Studies of Monolayers MoSi2N4 Decorated with Transition Metal Single-atom for Visible Light-driven High-efficient CO2 Reduction by Strain and Electronic Engineering. **2022**, 138198	2
296	Effect of disorder on thermodynamic instability of binary rare-earth □nickel □palladium compounds. **2022**, 118205	
295	Exploring the impact of lone pairs on the structural features of alkaline-earth (A) transition-metal (M,M′) chalcogenides (Q) AMM′Q3.	1
294	Zinc glycolate Zn(OCH2CH2O): synthesis and structure, spectral and optical properties, electronic structure and chemical bonding. **2022**, 166320	
293	Semiconductors with Chiral Crystal Structure in Group IVB Transition Metal Pernitrides.	0
292	Electronic Structure and Mechanical Properties of Ti5Si3. **2022**, 134, 743-753	1
291	Titanium Substitution Effects on the Structure, Activity, and Stability of Nanoscale Ruthenium Oxide Oxygen Evolution Electrocatalysts: Experimental and Computational Study. **2022**, 5, 11752-11775	0
290	Data-Driven Investigation of Tellurium-Containing Semiconductors for CO2 Reduction: Trends in Adsorption and Scaling Relations. **2022**, 126, 13224-13236	

289	A theoretical investigation of the effect of Ga alloying on thermodynamic stability, electronic-structure, and oxidation resistance of Ti2AlC MAX phase. **2022**, 12,	
288	Doping-stabilized Au-N compounds via lithium atoms at high pressure. **2022**, 4,	
287	Adsorption Site Preference Determined by Triangular Topology: Application of the Method of Moments to Transition Metal Surfaces. **2022**, 126, 13505-13519	1
286	Toward Computational Screening of Bimetallic Alloys for Methane Activation: A Case Study of MgPt Alloy. **2022**, 12, 9458-9472	3
285	The Orbital Nature of Electron Holes in BaFeO3 and Implications for Defect Chemistry. **2022**, 126, 12809-12819	1
284	Tunnel-structured willemite Zn2SiO4: Electronic structure, elastic, and thermal properties. **2022**, 11, 1249-1262	0
283	Nanotube Matrices for Flexible SnIP Nanowires. **2022**, 126, 12603-12614	
282	MgMn4Ga18: a novel three-shell gallium cluster structure. **2022**, 78, 455-461	
281	Enhancing Electrocatalytic Nitrogen Reduction on Few-Layer Antimonene in an Aqueous Potassium Sulfate Electrolyte. **2022**, 126, 13629-13639	1
280	Designing Inorganic Semiconductors with Cold-Rolling Processability. 2203776	0
279	High-Energy Ni-Rich LiNi0.85Co0.1Mn0.05O2 Cathode Material for Li-Ion Batteries Enhanced by Nd- and Y-Doping. A Structural, Electrochemical, and Thermal Investigation.	
278	Selective Chemical Substitution of Cu in the Structure of TiAl3 Type InPd3: Experimental and Theoretical Studies.	1
277	Prediction of super hardness in transition metal hexa-nitrides from density functional theory computations. **2022**, 101550	0
276	First-Principles Calculations of Two-Dimensional Monolayer PdSe2 for Selective Sensing of Nitrogen-Containing Gases. **2022**, 5, 11519-11528	0
275	Highly Strained Bi-MOF on Bismuth Oxyhalide Support with Tailored Intermediate Adsorption/Desorption Capability for Robust CO 2 Photoreduction.	2
274	Highly Strained Bi-MOF on Bismuth Oxyhalide Support with Tailored Intermediate Adsorption/Desorption Capability for Robust CO 2 Photoreduction.	
273	Equilibrium Particle Shape and Surface Chemistry of Disordered Li-Excess, Mn-Rich Li-ion Cathodes through First-Principles Modeling. **2022**, 34, 7210-7219	0
272	A single tiny Ti (O2) cluster decorated an ultra-small boron nitride nanotube for hydrogen storage material: A density functional theory study. **2022**,	0

271	Explaining the electronic band structure of half-Heusler thermoelectric semiconductors for engineering high valley degeneracy.	1
270	Evolution of Structural Properties in Fe Intercalated 2H-NbSe2: Phase Transformation Induced by Strong Host□Guest Interaction. **2022**, 126, 13762-13773	0
269	Stability Design Principles of Manganese-Based Oxides in Acid.	1
268	Anomalous bond softening mediated by strain-induced Friedel-like oscillations in a BC2N superlattice. **2022**, 106,	
267	Selective CO 2 Electroreduction to Ethanol over a Carbon-Coated CuO x Catalyst.	0
266	Computational study of transition metal single-atom catalysts supported on nitrogenated carbon nanotubes for electrocatalytic nitrogen reduction.	0
265	Function of Internal and External Fe in a Ni-Based Precatalyst System Toward Oxygen Evolution Reaction. **2022**, 61, 12772-12780	1
264	Selective CO 2 Electroreduction to Ethanol over a Carbon-Coated CuO x Catalyst.	1
263	Enhancing the thermionic electron emission performance of hafnium with nanocluster doping. **2022**, 121, 061603	
262	Cyclohexane and n-hexane adsorption studies on novel hex-star antimonene nanosheets □A first-principles outlook. **2022**, 144, 109823	1
261	Improving photoelectric perfomance with hydrogen on Al-doped ZnO. **2022**, 291, 126680	1
260	Synthesis and Characterization of New Multinary Selenides A 10 B 18 Se 37 (A=Sn/Pb; B=In/Sb/Bi).	0
259	Tunable electronic properties of diamond (100) surface via boron-nitrogen co-termination: A first-principles study. **2022**, 129, 109387	0
258	Rational design synergistic metal-free dual-atom electrocatalyst for N2 to NH3 reaction on g-CN: A first principle study. **2022**, 605, 154831	0
257	Coordination environment engineering of graphene-supported single/dual-Pd-site catalysts improves the electrocatalytic ORR activity. **2022**, 606, 154749	1
256	Highly sensitive and selective gas sensors based on nanoporous CN monolayer for reusable detection of NO, H2S and NH3: A first-principles study. **2022**, 606, 154806	0
255	Insights into Cation-disorder effect on stability, electronic structure and defect properties of Zn-IV-nitrides: The case of ZnGeN2. **2022**, 33, 104385	0
254	V8SiB4 □A new ternary phase in the V□Si□B system. **2022**, 151, 107691	0

253	Achieving high-energy and long-cycling aqueous zinc-metal batteries by highly reversible insertion mechanisms in Ti-substituted Na0.44MnO2 cathode. **2023**, 451, 139059	1
252	A descriptor for the design of 2D MXene hydrogen evolution reaction electrocatalysts. **2022**, 10, 18195-18205	0
251	Synthesis and structural characterization of the new Zintl phases Eu10Mn6Bi12 and Yb10Zn6Sb12. **2022**, 51, 13470-13478	0
250	bcc superstructures: RE2RuIn with RE = Sc, Y, Dy-Tm and Lu. **2022**, 51, 14156-14164	1
249	Bond activation and formation on inorganic surfaces. **2022**,	0
248	A 2D heavy fermion CePb3 kagome material on silicon: emergence of unique spin polarized states for spintronics.	0
247	The atomic defects on the (104) and (110) surfaces of the MgCl2-supported Ziegler-Natta Catalyst: a periodic DFT study.	1
246	An ab initio investigation of the temperature-dependent energetic barriers towards CrAlB and (Mo,Cr)AlB formation in a metastable synthesis scenario. **2022**, 14, 12866-12874	0
245	Crystal chemistry at high pressure. **2022**,	0
244	Interface-engineering studies on the photoelectric properties and stability of the CsSnI3/SnS heterostructure.	0
243	A theoretical roadmap for the best oxygen reduction activity in two-dimensional transition metal tellurides. **2022**, 13, 11048-11057	0
242	Effects of Aluminum Diffusion on the Oxide of the Fecral Alloys Surface: A First-Principles Study.	0
241	Tailoring interlayer magnetic coupling to modify the magnetic properties of FeCl2 bilayers by self-intercalation.	1
240	Water reduction on the facets of Fe(OH)2: an experimental and DFT study. **2022**, 9, 3407-3416	1
239	The role of Mo species in Ni-Mo catalysts for dry reforming of methane. **2022**, 24, 21461-21469	0
238	The "burst effect" of hydrogen desorption in MgH2 dehydrogenation.	2
237	Antibonding Induced Anharmonicity Leading to Ultralow Lattice Thermal Conductivity and Extraordinary Thermoelectric Performance in CsK2X (X = Sb, Bi).	0
236	Photoinduced CO2 and N2 reductions on plasmonically enabled gallium oxide. **2023**, 629, 654-666	0

235	Re nanoflower-decorated carbon cloth for pH-universal hydrogen evolution reaction: Unveiling the intrinsic electrocatalytic activity of metallic Re. **2023**, 452, 139461	0
234	Mg2MnGa3 □An orthorhombically distorted superstructure variant of the hexagonal Laves phase MgZn2. **2022**, 77, 727-733	1
233	Mg-Ni-Ga System: Phase Diagram, Structural and Hydrogenation Properties of MgNi1.25Ga0.75, MgNiGa, and Mg2NiGa3. **2022**, 43, 458-470	0
232	Discovery of Efficient Visible-light Driven Oxygen Evolution Photocatalysts: Automated High-Throughput Computational Screening of MA 2 Z 4. 2207415	4
231	Anchor single atom in h-BN assist NO synthesis NH3: a computational view. **2022**, 41, 3456-3465	1
230	Thermoelectric transport properties of XAgP (X = Sr and Ba) from first principles. **2022**, 34, 455501	0
229	Insights into the high-pressure behavior of solid bromine from hybrid density functional theory calculations. **2022**, 106,	0
228	ACuZrQ3 (A = Rb, Cs; Q = S, Se, Te): Direct Bandgap Semiconductors and Metals with Ultralow Thermal Conductivity. **2022**, 34, 8389-8402	0
227	Tuning Electronic Structure and Composition of FeNi Nanoalloys for Enhanced Oxygen Evolution Electrocatalysis via a General Synthesis Strategy. 2203340	0
226	Performance investigation of Ti x N x□O2 MXene (x = 2, 3, 4) as anode materials for Na-ion batteries by first-principles calculation. **2022**, 33, 495403	0
225	Oxidative Addition of Methane and Reductive Elimination of Ethane and Hydrogen on Surfaces: From Pure Metals to Single Atom Alloys.	0
224	The Crystal Structure of Carbonic Acid. **2022**, 10, 132	0
223	Softened sp2–sp3 bonding network leads to strong anharmonicity and weak hydrodynamics in graphene+. **2022**, 106,	2
222	Pressure induced decomposition of cadmium iodide.	0
221	Prediction of stability and lifetime of carbyne, carbyne–graphene and similar low-dimensional nanostructures.	0
220	Critical Role of Explicit Inclusion of Solvent and Electrode Potential in the Electrochemical Description of Nitrogen Reduction. **2022**, 12, 11530-11540	1
219	Stabilization of A -site ordered perovskites and formation of spin-half antiferromagnetic lattice: CaCu3Ti4O12 and . **2022**, 106,	0
218	Self-Passivated Metal Klein Edge of 1T-Phase Transition Metal Dichalcogenides and the Induced High-Efficient Hydrogen Evolution Reaction Activity. 2208414	1

217	Impeded degradation of perovskite solar cells via the dual interfacial modification of siloxane.	0
216	Lattice strain and band overlap of the thermoelectric composite Mg2Si1−xSnx. **2022**, 106,	0
215	Single Iron-dimer Catalysts on MoS2 Nanosheet for Potential Nitrogen Activation.	0
214	The Exotically Stoichiometric Compounds and Superconductivity of Lithium–Copper Systems under High Pressure. 9250-9254	0
213	Enhanced oxygen evolution over dual corner-shared cobalt tetrahedra. **2022**, 13,	4
212	Analysis of grain boundary embrittlement by Cu and Sn in paramagnetic Fe by first-principles computational tensile test. **2022**, 6,	0
211	Pressure-induced novel structure with graphene-like boron-layer in titanium monoboride.	0
210	Enhanced ionic conductivity and lack of paddle-wheel effect in pseudohalogen-substituted Li argyrodites. **2022**,	1
209	Dynamics of non-metal-regulated FeCo bimetal microenvironment on oxygen reduction reaction activity and intrinsic mechanism.	0
208	Orbital Orientation-based Theoretical Design of Single-Atom Catalysts for the Hydrogen Evolution Reaction. **2022**, 126, 16656-16662	0
207	Termolecular Eley–Rideal pathway for efficient CO oxidation on phosphorene-supported single-atom cobalt catalyst.	0
206	Vacancy diffusion on a brominated Si(100) surface: Critical effect of the dangling bond charge state. **2022**, 157, 124705	0
205	Identification of the Intrinsic Active Site in Phase-Pure M1 Catalysts for Oxidation Dehydrogenation of Ethane by Density Functional Theory Calculations.	0
204	Optoelectronic and photocatalytic properties of Mo-based Janus monolayers for solar cell applications. **2022**, 170071	0
203	Enhanced Electrocatalytic CO2 Conversion to CH4 via Molecular Engineering on Copper Salphen Complexes.	0
202	Effects of aluminum diffusion on the oxide of the FeCrAl alloys surface: A first–principles study. **2022**, 104594	0
201	Crystalline aluminum silicides with electride state and superconductivity under high pressure. **2022**, 28, 100853	0
200	Investigation of hardness in transition metal hexa-nitrides in cubic structure: A first-principles study. **2022**, 171, 111022	0

199	Formulating electronic descriptors to rationally design graphene-supported single-atom catalysts for oxygen electrocatalysis.	0
198	Magnetic materials. **2022**,	0
197	GaPS2Se2 Monolayer: Novel Stable 2D Janus Semiconductor with Anisotropic Properties for Spontaneous Water splitting under the Irradiation of Solar Light.	0
196	Prediction of stable silver selenide-based energy materials sustained by rubidium selenide alloying.	0
195	Chemical Bonding With Plane Waves. **2022**,	0
194	Shear adhesive strength between epoxy resin and copper surfaces: a density functional theory study.	1
193	Electronic Properties and Chemical Bonding in V2FeSi and Fe2VSi Heusler Alloys. **2022**, 12, 1546	1
192	26.2: Invited Paper: Computational chemistry study of an aggregation-induced delayed fluorescence material: synthesis and properties. **2022**, 53, 286-299	0
191	Revealing the effect of Ni NPs on the ignition characteristics of Al/ethanol nanofluid fuel: Experimental and DFT insights. **2022**, 155508	0
190	Fe□NC Boosts the Stability of Supported Platinum Nanoparticles for Fuel Cells.	3
189	Polymeric Hydronitrogen N4H: A Promising High-Energy-Density Material and High-Temperature Superconductor.	0
188	Origin of ferroelectricity in magnesium-doped zinc oxide. **2022**, 106,	1
187	Chemical Pressure-Derived Assembly Principles for Dodecagonal Quasicrystal Approximants and Other Complex Frank□Kasper Phases.	0
186	Experimental Study of Diamond-like Carbon Film on Aermet100 Steel and First-Principles Calculation of Interfacial Adhesion. **2022**, 14, 48262-48275	0
185	Synthetic Engineering in Na2MSn2(NCN)6 (M = Mn, Fe, Co, and Ni) Based on Electronic Structure Theory.	2
184	The effect of solute segregation on stability and strength of Cu symmetrical tilt grain boundaries from the first-principles study. **2022**,	0
183	Mo-Doped Metal□Organic Frameworks for Efficient Nitrogen Reduction Reaction: A Density Functional Theory Study. **2022**, 10, 14064-14072	1
182	d-Orbital-Driven Low Lattice Thermal Conductivity in TiRhBi: A Root for Potential Thermoelectric and Microelectronic Performance.	0

181	Inhibiting Sulfur Dissolution and Enhancing Activity of SnS for CO2 Electroreduction via Electronic State Modulation. 13533-13541	5
180	Stability of and conduction in single-walled Si2BN nanotubes. **2022**, 6,	0
179	Understanding the Difference in Bulk Modulus between Y-doped SrCeO3 and Y-doped SrZrO3 by Ultrasonic Transmission Method and Density Functional Theory. **2022**, 101616	0
178	MNBr (M = Mo, Cr, V) monolayer: two-dimensional ferromagnetic half-metallic materials with high Curie temperature. **2022**, 55, 505002	0
177	Y2Mo3O12Ba0.5Sr0.5Co0.8Fe0.2O3-δ cathode catalyst for proton-conducting solid oxide fuel cells. **2022**, 551, 232073	0
176	First principle studies on electronic and thermoelectric properties of Fe2TiSn based multinary Heusler alloys. **2023**, 216, 111856	0
175	Structural screening and descriptor exploration of black phosphorus carbide supported bifunctional catalysts for lithium-sulfur batteries. **2023**, 630, 317-327	0
174	Optimal doping elements for inhibiting surface-diffusion of adatoms on Cu3Sn. **2023**, 609, 155003	0
173	Theoretical Investigation of Single-Atom Catalysts Anchored on Pure Carbon Substrate for Electroreduction of NO to NH3.	0
172	Four ternary silicides in the La–Ni–Si system: from polyanionic layers to frameworks.	0
171	Trends in opto-electronic properties of MgxZn1-xSnN2 using first principles methods. **2023**, 294, 126995	0
170	Improving the ORR Performance by Enhancing the Pt Oxidation Resistance. **2022**,	0
169	Photocatalytic and Photocurrent Responses to Visible Light of the Lone-Pair-Based Oxysulfide Sr6Cd2Sb6S10O7.	0
168	A crystal glass–nanostructured Al-based electrocatalyst for hydrogen evolution reaction. **2022**, 8,	2
167	Strain-Tuneable Magnetism and Spintronics of Distorted Monovacancies in Graphene. **2022**, 126, 19435-19445	0
166	DFT study on TiO2 facet-dependent As(III) oxidation process: Importance of As(IV) species. **2022**, 122219	0
165	Investigation and understanding of the mechanical properties of MXene by high-throughput computations and interpretable machine learning. **2022**, 101921	0
164	Breaking the Volcano-Shaped Relationship for Highly Efficient Electrocatalytic Nitrogen Reduction: A Computational Guideline.	0

163	Computational Insight into Defective Boron Nitride Supported Double-Atom Catalysts for Electrochemical Nitrogen Reduction. **2022**, 12, 1404	0
162	Exploring the subtle factors that control the structural preferences in Cu7Te4.	1
161	Electron Counting and High-Pressure Phase Transformations in Metal Hexaborides.	0
160	Chemical templates that assemble the metal superhydrides. **2022**,	0
159	Unveiling Chemically Robust Bimetallic Squarate-Based Metal□Organic Frameworks for Electrocatalytic Oxygen Evolution Reaction. 2202964	0
158	The optimal tuning of electronic structure, magnetic, and optical properties of (Fe, V + VO/ VSn) co-doped SnO2 via first-principles calculations.	0
157	Impact of vacancies on structure, stability and properties of hexagonal transition metal diborides, MB2 (M = Sc, Y, Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W, Mn, and Fe). **2022**, 101629	0
156	Single-layer MoS2 with adjacent Mo sites for efficient electrocatalytic nitrogen fixation via spin-delocalized electrons effect. **2023**, 323, 122186	1
155	Na2Mn(CO3)2: A carbonate based prototype cathode material for Na-ion batteries with high rate capability □An ab-initio study. **2023**, 439, 141687	0
154	Theoretical insight into electrocatalytic nitrogen fixation on transition-metal decorated melon-based carbon nitride. **2023**, 535, 112862	0
153	Extracellular polymeric substances enhance dissolution and microbial methylation of mercury sulfide minerals.	0
152	<i>Ab Initio</i> Local-Energy and Local-Stress Calculations for Materials Science and Engineering. **2023**, 87, 1-17	0
151	Adjusting OH tolerance of Ni4 clusters supported on ultra-small carbon nanotube with lattice vacancies for hydrogen oxidation catalysts. **2023**, 27, 101262	0
150	A computational study on CO2 electrochemical reduction on two dimensional metal-1,2,3,4,5,6,7,8,9,10,11,12-perthiolated coronene frameworks.	0
149	Effect of Mo addition on hydrogen segregation at □-Fe grain boundaries: A first-principles investigation of the mechanism by which Mo addition improves hydrogen embrittlement resistance in high-strength steels. **2023**, 218, 111951	0
148	Understanding the origins of low lattice thermal conductivity in a novel two-dimensional monolayer NaCuS for achieving medium-temperature thermoelectric applications. **2023**, 614, 156167	0
147	Achieving highest Young's modulus in Al-Li by tracing the size and bonding evolution of Li-rich precipitates. **2023**, 145, 125-135	0
146	Highly selective production of singlet oxygen by manipulating the spin state of single-atom Co□N moieties and electron localization. **2023**, 324, 122248	0

145	Localization versus delocalization of d-states within the $$hbox {Ni}_{{2}}$$MnGa Heusler alloy. **2022**, 12,	1
144	Magic Sinter-Resistant Cluster Sizes of Ptn Supported on Alumina. **2022**, 13, 11044-11050	1
143	Super-exchange effect induced by early 3d metal doping on NiFe2O4(001) surface for oxygen evolution reaction. **2022**,	0
142	Influence of germanium substitution on the structural and electronic stability of the competing vanadium dioxide phases. **2022**, 4,	0
141	Controlled Synthesis of Palladium Phosphides with Tunable Crystal Phases and Their Sulfur-Tolerant Performance. **2022**, 12, 15193-15206	1
140	On the Nature of Three-Atom Metal Cluster Catalysis for N2 Reduction to Ammonia. **2022**, 12, 14964-14975	1
139	Elemental segregation inhibits hydrogen embrittlement in aluminium alloys. **2022**, 100099	0
138	Design of Single-Atom Catalysts for Hg0 Oxidation Using H2O2. **2022**, 126, 21234-21242	0
137	Sn(IV) Polyanionic Materials as Efficient Visible-Light-Driven Water-Splitting Photocatalysts. **2022**, 126, 21243-21252	0
136	Prediction of erbium nitrogen compounds as high-performance high-energy-density materials. **2023**, 35, 085701	0
135	Regulating the metal-support interactions by tuning the ratios between N and B based on the C2N motif to develop efficient Pd-based catalysts for CO oxidative coupling to DMO: A DFT study. **2022**, 156205	0
134	Design principles for transition metal nitride stability and ammonia generation in acid. **2022**,	0
133	Diameter-Dependent Ultrafast Lithium-Ion Transport in Carbon Nanotubes.	0
132	Lutetium-Doped ZnO to Improve Photovoltaic Performance: A First-Principles Study. **2022**, 4, 6253-6260	0
131	In Quest of Low-Leakage Dynamic Random Access Memory Enabled by Doped TiO 2 Dielectrics. 2200614	1
130	Orbital Modulation with P Doping Improves Acid and Alkaline Hydrogen Evolution Reaction of MoS2. **2022**, 12, 4273	0
129	High-throughput theoretical optimization of the selective reduction reaction of NO with NH3 on metal-organic frameworks. **2022**, 122238	0
128	Are Janus MoSSe/Ti3C2-MXene heterostructures excellent anode materials for Na-ion batteries? A computational insight combined experiment. **2022**, 156196	0

127	Enhanced magnetism in Ru-doped hybrid improper perovskite Ca 3 Mn 2 O 7 via experimental and first-principles study.	0
126	Photolysis versus Photothermolysis of N2O on a Semiconductor Surface Revealed by Nonadiabatic Molecular Dynamics.	3
125	Revisiting the Nature of Chemical Bonding in Chalcogenides to Explain and Design their Properties. 2208485	1
124	MAl4Ir2 (M = Ca, Sr, Eu): superstructures of the KAu4In2 type.	0
123	Biphenylene Network as Sodium Ion Battery Anode Material.	0
122	Magnetic molecular orbitals in MnSi. **2023**, 9,	0
121	KOH-Enabled Axial-Oxygen Coordinated Ni Single-Atom Catalyst for Efficient Electrocatalytic CO 2 Reduction. 2201311	0
120	Cu-Doped MoSi 2 N 4 Monolayer as a Potential NH 3 Sensor.	0
119	Electrocatalysis Mechanism and Structure–Activity Relationship of Atomically Dispersed Metal-Nitrogen-Carbon Catalysts for Electrocatalytic Reactions. 2201524	0
118	Got Coke? Self-Limiting Poisoning Makes an Ultra Stable and Selective Sub-Nano Cluster Catalyst. 1533-1544	2
117	Long Distance Bimetallic Site in Crystal with Relay Metal-N-N-Metal Mechanism and New Descriptors for Electrocatalytic Nitrogen Reduction Reaction. **2023**, 119030	0
116	Emergent Transitions: Discord between Electronic and Chemical Pressure Effects in the REAl3 (RE = Sc, Y, Lanthanides) Series.	0
115	Enhancement of CO adsorption energy on defective graphene-supported Cu13 cluster and prediction with an induction energy model. **2023**, 156368	0
114	On the atomistic origin of the polymorphism and the dielectric physical properties of beryllium oxide.	0
113	Strong Antibonding I (p)–Cu (d) States Lead to Intrinsically Low Thermal Conductivity in CuBiI4. **2023**, 145, 1349-1358	0
112	Cu4TiTe4: Synthesis, Crystal Structure, and Chemical Bonding. **2023**, 62, 748-755	0
111	Low-cost, high-density MnCo spinel coatings for stainless steel interconnect via efficient microwave heating. **2023**, 136107	0
110	Clathrate-Like Alkali and Alkaline-Earth Metal Borides: A New Family of Superconductors with Superior Hardness. 2213377	0

109	Hydrogen-Bond-Promoted ORR Mechanism in P-Doped Fe□□ Materials.	0
108	Mechanochemistry and the Evolution of Ionic Bonds in Dense Silver Iodide.	0
107	The Importance of Mg□b Interactions in Achieving High Conduction Band Degeneracy in Mg3Sb2 for High n-Type Thermoelectric Performance. **2023**, 31, 100959	0
106	An unexpectedly stable Y2B5 compound with the fractional stoichiometry under ambient pressure. **2023**, 16, 104546	0
105	Investigation on the electronic structures, elastic and thermodynamic properties of TiNi, Ti2Ni and TiNi3 intermetallic compound. **2023**, 34, 105273	1
104	Functionalized Mo2BX2 (X = H, OH, O) MBenes as a promising sensor, capturer and storage material for environmentally toxic gases: A case. **2023**, 615, 156299	0
103	Computational screening of two-dimensional substrates for stabilizing honeycomb borophene. **2023**, 615, 156388	0
102	Machine-Learning-Assisted Discovery of High-Efficient Oxygen Evolution Electrocatalysts. **2023**, 14, 170-177	0
101	ELECTRONIC STRUCTURE, CHEMICAL BONDING, AND PHASE STABILITY OF THORIUM BORIDES ThB4, ThB6 AND ThB12. **2022**, 63, 1943-1948	0
100	Suppressing initial capacity fade in Li-rich Li5FeO4 with anionic redox by partial Co substitution - a first-principles study.	0
99	Accidental persistent spin textures in the proustite mineral family. **2023**, 107,	0
98	Exploring the Interdependence between Electronically Unfavorable Situations and Pressure in a Chalcogenide Superconductor. **2023**, 11, 61	0
97	Dynamic Lone Pair Expression as Chemical Bonding Origin of Giant Phonon Anharmonicity in Thermoelectric InTe.	0
96	Abnormal behavior of preferred formation of the cationic vacancies from the interior in a □GeSe monolayer with the stereo-chemical antibonding lone-pair state.	0
95	Fascinating Electrocatalysts with Dispersed Di-Metals in MN 3 -M?N 4 Moiety as Two Active Sites Separately for N 2 and CO 2 Reduction Reactions and Jointly for C?N Coupling and Urea Production. 2201331	0
94	Dual Function of Hypo-d-electronic Transition Metals in the Brewer Intermetallic Phase for the Highly Efficient Electrocatalytic Hydrogen Evolution Reaction in Alkaline Electrolytes. **2023**, 62, 2188-2196	0
93	Stability and Elasticity of Quasi-Hexagonal Fullerene Monolayer from First-Principles Study. **2023**, 13, 224	1
92	Theoretical exploration of the origin of selectivity for the oxidative carbonylation reaction catalyzed by a single Pd atom embedded on graphene.	0

91	Charting Ba-Based Double Perovskite Oxides for Visible-Light-Driven Photocatalytic Water Splitting. **2023**, 127, 3968-3976	0
90	Redox Promotion by Prelithiation Modification of the Separator in Lithium–Sulfur Batteries. **2023**, 127, 4006-4014	0
89	Synthesis and Characterization of Multinary Selenides A 4 B 10 Se 19 (A=Sn, Pb; B=Sb, Bi). **2023**, 649,	0
88	Precise Electronic Structures of Amorphous Solids: Unraveling the Color Origin and Photocatalysis of Black Titania.	0
87	Understanding formation of the InPd3 polymorphs: a DFT study. **2023**,	0
86	First-principles design of highly active and durable Ti55Cx@Pt92 nanocatalyst for oxygen reduction reaction through charge control at nanointerfaces. **2023**, 618, 156685	0
85	Electronic structure exquisite modulation of NiSe2 interface via rationally controlling Fe doping for boosting electrochemical oxygen evolution activity. **2023**, 464, 142620	0
84	Syngas-to-C2 oxygenates over the inverse Mo6C4/Cu catalyst: Identifying the role of synergistic effect. **2023**, 619, 156746	0
83	Structural phase stability and thermodynamical properties of transition metal complex hydrides Na2MgTMH7 (TM=Sc–Cu) for hydrogen storage applications. **2023**, 321, 123867	0
82	Ethylene carbonate generated efficiently via ethylene oxide and CO2 on the Li-MgO(1 0 0) surface based on the synergistic activation of bimetals without halogen. **2023**, 342, 127823	0
81	Theoretical design toward highly efficient single-atom catalysts for nitrogen reduction by regulating the “acceptance-donation” mechanism. **2023**, 623, 156827	0
80	CaPt4P6, first calcium-containing representative of the ternary pyrite-derived pnictides of the BaPt4As6 type: Synthesis, crystal, and electronic structure. **2023**, 322, 123969	0
79	Discerning the crystal structure and engineering the optoelectronic properties through substitution of divalent cations (M= Zn, N = Ge) in C3H3MNI3 for solar cell applications. **2023**, 160, 107449	0
78	Robust magnetism of the cluster assembled (Fe@In6)Ba2 crystal. **2023**, 1224, 114106	0
77	Effects of transition metal segregation on the thermodynamic stability and strength of Ni Σ11 [110](113) symmetrical tilt grain boundary. **2023**, 212, 112036	0
76	Coral-shaped Mn-CuS with hierarchical pores and crystalline defects for high-efficiency H2O2 production via electrocatalytic two-electron reduction. **2023**, 331, 122721	0
75	Investigation on transport properties and anomalously heat-carrying optical phonons in KXY (X = Ca, Mg; Y = Sb, Bi). **2023**, 209, 124132	0
74	Electronic structure of the magnetic halide double perovskites Cs2(Ag,Na)FeCl6 from first principles. **2023**, 7,	0

73	Understanding the hydrogen evolution reaction activity of doped single-atom catalysts on two-dimensional GaPS4 by DFT and machine learning. **2023**, 81, 93-100	0
72	Computational design of one FeCoNiCuZn high-entropy alloy for high-performance electrocatalytic nitrate reduction. **2023**, 626, 157246	0
71	First-principles calculations investigation on different coverage of H2O adsorption on the Mg-montmorillonite (0 1 0) edge surface. **2023**, 626, 157232	0
70	In-situ surface reconstruction of single-crystal (NiFe)3Se4 nano-pyramid arrays for efficient oxygen evolution. **2023**, 642, 532-539	0
69	Electrocatalytic hydrogen evolution on the MoS2/C60 heterostructure: Reaction mechanism and activity improvement. **2023**, 624, 157163	0
68	Computational studies for boosting nitrate electroreduction activity of Fe-N4-C Single-Atom catalyst via axial fifth ligand. **2023**, 616, 156440	0
67	Theoretical screening of synergistic transition metal dual-atom catalysts for overall water splitting. **2023**, 220, 112034	0
66	Dynamic Lone Pair Expression as Chemical Bonding Origin of Giant Phonon Anharmonicity in Thermoelectric InTe. **2023**, 135,	0
65	Screening of single-atom catalysts of transition metal supported on MoSe2 for high-efficiency nitrogen reduction reaction. **2023**, 537, 112967	1
64	Emerging d□ orbital coupling between non-d-block main-group elements Mg and I at high pressure. **2023**, 26, 106113	0
63	Electric-field-tunable thermal conductivity in anti-ferroelectric materials. **2023**, 32, 100998	0
62	Orthorhombic Na2/3Cu0.1Mn0.9O2 cathode: Enhanced Na storage performances with the suppressed Mn□ bond anisotropy. **2023**, 460, 141744	0
61	Terminal Atom-Controlled Etching of 2D-TMDs. 2211252	0
60	Synthesis of technetium hydride TcH1.3 at 27 GPa. **2023**, 107,	0
59	Boosting Oxygen Electrocatalytic Activity of Fe□□ Catalysts by Phosphorus Incorporation. **2023**, 145, 3647-3655	0
58	Single-phase lightweight high-entropy alloys with enhanced mechanical properties. **2023**, 227, 111709	0
57	Potential rules for stable transition metal hexafluorides with high oxidation states under high pressures. **2023**, 25, 6726-6732	0
56	Metal-Free Carbon Nitride Nanosheet Supported the Pentacoordinated Silicon Intermediates for Photocatalytic Overall Water Splitting. **2023**, 14, 1918-1927	0

55	Proton migration barriers in BaFeO3 Insights from DFT calculations. **2023**, 11, 6336-6348	0
54	New Trick for an Old Dog: From Prediction to Properties of Hidden Clathrates Ba2Zn5As6 and Ba2Zn5Sb6. **2023**, 145, 4638-4646	0
53	First-principles study for discovery of novel synthesizable 2D high-entropy transition metal carbides (MXenes). **2023**, 11, 5681-5695	0
52	First Principles Study of Atomic Oxygen Adsorption on Austenitic Stainless Steels Surfaces: A Theoretical Study. **2023**, 13, 455	0
51	Revealing hidden phases and self-healing in antimony trichalcogenides and chalcoiodides. **2023**, 4, 101298	0
50	Identifying the ground state structures of point defects in solids. **2023**, 9,	0
49	First-principle insights of initial hydration behavior affected by copper impurity in alite phase based on static and molecular dynamics calculations. **2023**, 398, 136478	0
48	Mechanical and electronic properties of transition metal hexa-nitrides in hexagonal structure from density functional theory calculations. **2023**, 221, 112084	0
47	DFT-Based Study for the Enhancement of CO2 Adsorption on Metal-Doped Nitrogen-Enriched Polytriazines. **2023**, 8, 8876-8884	0
46	Solution-Phase Synthesis and Photoluminescence of Quaternary Chalcohalide Semiconductors. **2023**, 35, 2165-2172	0
45	Origin of contrasting trends of intrinsic electron mobility with tensile strain in hexagonal MoS2 and triangular PdSe2. **2023**, 107,	0
44	Superconducting H7 chain in gallium hydrides at high pressure. **2023**, 25, 7223-7228	0
43	Effects of NH4+ doping on the hydrogen storage properties of metal hydrides. **2023**,	0
42	Stable Rb-B compounds under high pressure. **2023**, 5,	0
41	Tiny (ZnO) clusters supported on graphene for solar energy trapping: A density functional theory study. **2023**, 144, 104769	0
40	The decisive role of adsorbed OH* in low-potential CO electro-oxidation on single-atom catalytic sites.	0
39	Chemical bonding engineering for high-symmetry Cu2S-based materials with high thermoelectric performance. **2023**, 32, 101028	0
38	Catalytic CO Oxidation by Single Atom Catalysts of Transition Metal-doped -Borophene: A First Principles Study. **2023**, 52, 249-253	0

37	Change in the Electronic Environment of the VOx Active Center via Support Modification to Enhance Hg Oxidation Activity. **2023**, 13, 3775-3787	0
36	Potential-Dependent Oxygen Reduction on FeN4 under Explicit Solvation Environment. **2023**, 127, 4934-4941	0
35	Interfacial contact barrier and charge carrier transport of MoS2/metal(001) heterostructures. **2023**, 25, 9548-9558	0
34	Eu4Al13Pt9 a coloring variant of the Ho4Ir13Ge9 type structure. **2023**, 78, 147-156	0
33	First-Principles Study of the Effects of Ti Content on Mechanical Properties and Microscopic Mechanism in Cu2AlMn1 Tix Alloys. **2023**, 13, 466	0
32	Valence Band Structure Degeneracy Enhanced Thermoelectric Performance in Cu2Se. **2023**, 127, 5576-5583	0
31	Engineering the catalytic properties of CeO2 catalyst in HCl-assisted propane dehydrogenation by effective doping: A first-principles-based microkinetic simulation. 11,	0
30	Modulating the Combinatorial Target Power of MgSnN2 via RF Magnetron Sputtering for Enhanced Optoelectronic Performance: Mechanistic Insights from DFT Studies.	0
29	Promoter Poison Partnership Protects Platinum Performance in Coked Cluster Catalysts. **2023**, 127, 5376-5384	0
28	Theoretical study on hydrogen evolution reaction in transition metal borides.	0
27	Computational Design and Theoretical Properties of WC3N6, an H-Free Melaminate and Potential Multifunctional Material. **2023**, 145, 6986-6993	0
26	The charge effects on the hydrogen evolution reaction activity of the defected monolayer MoS2. **2023**, 25, 10956-10965	0
25	Deformation mechanism of L12-type multicomponent intermetallics: The generalized stacking fault energy and chemical bonds. **2023**, 228, 111824	0
24	Precise electronic structure modulation on MXene-based single atom catalysts for high-performance electrocatalytic CO2 reduction reaction: A first-principle study. **2023**, 642, 273-282	0
23	PtTe2/Sb2S3 Nanoscale Heterostructures for the Photocatalytic Direct Z-Scheme with High Solar-to-Hydrogen Efficiency: A Theoretical Investigation. **2023**, 6, 5591-5601	0
22	Activation of NO 2 by Modifying the Porphyrin Unit with Oxygen in a MnN 4 Graphene Layer. **2023**, 8,	0
21	Enhanced desulfurization performance of copper aerogel-based absorbents. **2023**, 40, 791-801	0
20	Designing single-site alloy catalysts using a degree-of-isolation descriptor.	0

19	Pressure-induced electride phase formation in calcium: A key to its strange high-pressure behavior. **2023**, 107,	0
18	Experimental and Theoretical Investigations of Out-of-Plane Ordered Nanolaminate Transition Metal Borides: M4CrSiB2 (M = Mo, W, Nb). **2023**, 62, 5341-5347	0
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16	Correlation of the spin state and catalytic property of MN4 single-atom catalysts in oxygen reduction reactions.	0
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9	A quasi-one-dimensional bulk thermoelectrics with high performance near room temperature. **2023** ,	0
8	MatHub-2d: A database for transport in 2D materials and a demonstration of high-throughput computational screening for high-mobility 2D semiconducting materials.	0
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3	Structural control of heterostructured Co3N-Co nano-corals for boosting electrocatalytic hydrogen evolution based on insulator-confined plasma engineering. **2023**, 466, 143211	0
2	From Laves Phases to Quasicrystal Approximants in the NaAuCd System. **2023**, 62, 6873-6881	0

1	Pressure-induced antiferromagnetic-tetragonal to nonmagnetic-collapse-tetragonal insulator-metal transition in ThMnAsN.	0