Myung-Hwan Whangbo

List of Publications by Citations

285 papers	9,386 citations	50 h-index	88 g-index
308 ext. papers	10,451 ext. citations	6.1 avg, IF	6.18 L-index

#	Paper	IF	Citations
285	Facile in situ synthesis of visible-light plasmonic photocatalysts M@TiO2 (M = Au, Pt, Ag) and evaluation of their photocatalytic oxidation of benzene to phenol. *Journal of Materials Chemistry*, **2011**, 21, 9079		494
284	Organic superconductors--new benchmarks. *Science*, **1991**, 252, 1501-8	33.3	332
283	Factors Affecting the Height and Phase Images in Tapping Mode Atomic Force Microscopy. Study of Phase-Separated Polymer Blends of Poly(ethene-co-styrene) and Poly(2,6-dimethyl-1,4-phenylene oxide). *Langmuir*, **1997**, 13, 3807-3812	4	278
282	**2013**,		258
281	Spin exchange interactions and magnetic structures of extended magnetic solids with localized spins: theoretical descriptions on formal, quantitative and qualitative levels. *Journal of Solid State Chemistry*, **2003**, 176, 417-481	3.3	254
280	Magnetic properties and energy-mapping analysis. *Dalton Transactions*, **2013**, 42, 823-53	4.3	215
279	Tunable ferroelectric polarization and its interplay with spin-orbit coupling in tin iodide perovskites. *Nature Communications*, **2014**, 5, 5900	17.4	215
278	Composite of CH NH PbI with Reduced Graphene Oxide as a Highly Efficient and Stable Visible-Light Photocatalyst for Hydrogen Evolution in Aqueous HI Solution. *Advanced Materials*, **2018**, 30, 1704342	24	213
277	Formulation of Phosphorescence Mechanisms in Inorganic Solids Based on a New Model of Defect Conglomeration. *Chemistry of Materials*, **2006**, 18, 3212-3220	9.6	202
276	Rational Design of Synthetic Metal Superconductors. *Progress in Inorganic Chemistry*,51-218		169
275	Predicting the spin-lattice order of frustrated systems from first principles. *Physical Review B*, **2011**, 84,	3.3	166
274	Spin-Hamiltonian and density functional theory descriptions of spin exchange interactions. *Journal of Chemical Physics*, **2001**, 114, 2887-2893	3.9	161
273	Spin-orbit coupling and ion displacements in multiferroic TbMnO3. *Physical Review Letters*, **2008**, 101, 037209	7.4	158
272	Spin exchange interactions of a spin dimer: Analysis of broken-symmetry spin states in terms of the eigenstates of Heisenberg and Ising spin Hamiltonians. *Journal of Chemical Physics*, **2003**, 118, 29-39	3.9	154
271	On the Factors Affecting the Contrast of Height and Phase Images in Tapping Mode Atomic Force Microscopy. *Langmuir*, **1997**, 13, 6349-6353	4	146
270	Synthesis and characterization of ZnS with controlled amount of S vacancies for photocatalytic H2 production under visible light. *Scientific Reports*, **2015**, 5, 8544	4.9	137
269	Ni Coordination to an Al-Based Metal-Organic Framework Made from 2-Aminoterephthalate for Photocatalytic Overall Water Splitting. *Angewandte Chemie - International Edition*, **2017**, 56, 3036-3040	16.4	128

268	Origin of the structural and magnetic anomalies of the layered compound SrFeO2: a density functional investigation. *Physical Review Letters*, **2008**, 100, 167207	7.4	126
267	On the possibility of ferromagnetism in carbon-doped anatase TiO2. *Applied Physics Letters*, **2008**, 93, 132507	3.4	124
266	Hole density dependence of the critical temperature and coupling constant in the cuprate superconductors. *Science*, **1990**, 249, 1143-6	33.3	123
265	Emergence of ferroelectricity and spin-valley properties in two-dimensional honeycomb binary compounds. *Physical Review B*, **2015**, 91,	3.3	107
264	Enhancing the Photocatalytic Hydrogen Evolution Activity of Mixed-Halide Perovskite CH3NH3PbBr3−xIx Achieved by Bandgap Funneling of Charge Carriers. *ACS Catalysis*, **2018**, 8, 10349-10357	13.1	106
263	Ferromagnetism of undoped GaN mediated by through-bond spin polarization between nitrogen dangling bonds. *Applied Physics Letters*, **2009**, 94, 162505	3.4	105
262	Ag6Si2O7: a Silicate Photocatalyst for the Visible Region. *Chemistry of Materials*, **2014**, 26, 3873-3875	9.6	104
261	Effects of spin-orbit coupling on magnetic properties of discrete and extended magnetic systems. *Journal of Computational Chemistry*, **2008**, 29, 2187-209	3.5	102
260	Characterization of the Morphologies and Nanostructures of Blends of Poly(styrene)-block-poly(ethene-co-but-1-ene)-block-poly(styrene) with Isotactic and Atactic Polypropylenes by Tapping-Mode Atomic Force Microscopy. *Langmuir*, **1998**, 14, 1219-1226	4	100
259	CuO Nanoparticles with Both {100} and {111} Facets for Enhancing the Selectivity and Activity of CO Electroreduction to Ethylene. *Advanced Science*, **2020**, 7, 1902820	13.6	97
258	Magnetic ordering in the frustrated Heisenberg chain system cupric chloride CuCl2. *Physical Review B*, **2009**, 80,	3.3	96
257	Strong Dzyaloshinskii-Moriya interaction and origin of ferroelectricity in Cu2OSeO3. *Physical Review Letters*, **2012**, 109, 107203	7.4	95
256	Giant ferroelectric polarization of CaMn7O12 induced by a combined effect of Dzyaloshinskii-Moriya interaction and exchange striction. *Physical Review Letters*, **2012**, 108, 187204	7.4	92
255	Consequences of a linear two-coordinate geometry for the orbital magnetism and Jahn-Teller distortion behavior of the high spin iron(II) complex Fe[N(t-Bu)2]2. *Journal of the American Chemical Society*, **2009**, 131, 404-5	16.4	90
254	Interpreting STM and AFM Images. *Advanced Materials*, **1994**, 6, 355-371	24	90
253	Structural Model of Planar Defects in CaCu3Ti4O12Exhibiting a Giant Dielectric Constant. *Chemistry of Materials*, **2006**, 18, 3257-3260	9.6	89
252	Perovskite photocatalyst CsPbBr3-xIx with a bandgap funnel structure for H2 evolution under visible light. *Applied Catalysis B: Environmental*, **2019**, 245, 522-527	21.8	82
251	Density-functional characterization of the multiferroicity in spin spiral chain cuprates. *Physical Review Letters*, **2007**, 99, 257203	7.4	80

250	Classical spin and quantum-mechanical descriptions of geometric spin frustration. *Journal of Chemical Physics*, **2004**, 121, 672-80	3.9	74
249	Cooperative effect of electron correlation and spin-orbit coupling on the electronic and magnetic properties of Ba2NaOsO6. *Physical Review B*, **2007**, 75,	3.3	73
248	Enhancing the Thermoelectric Properties of Layered Transition-Metal Dichalcogenides 2H-MQ2 (M = Mo, W; Q = S, Se, Te) by Layer Mixing: Density Functional Investigation. *Chemistry of Materials*, **2013**, 25, 3745-3752	9.6	72
247	Interplay between Jahn-Teller instability, uniaxial magnetism, and ferroelectricity in Ca3CoMnO6. *Physical Review B*, **2009**, 79,	3.3	65
246	CuBr2--a new multiferroic material with high critical temperature. *Advanced Materials*, **2012**, 24, 2469-73	24	61
245	Possibility of combining ferroelectricity and Rashba-like spin splitting in monolayers of the 1T-type transition-metal dichalcogenides MX2(M=Mo,W;X=S,Se,Te). *Physical Review B*, **2016**, 94,	3.3	59
244	Scanning Force Microscopy Study of Patterned Monolayers of Alkanethiols on Gold. Importance of Tip□Sample Contact Area in Interpreting Force Modulation and Friction Force Microscopy Images. *Langmuir*, **1997**, 13, 373-377	4	59
243	Strain-induced quantum spin Hall effect in methyl-substituted germanane GeCH3. *Scientific Reports* , **2014**, 4, 7297	4.9	58
242	Analysis of the uniaxial magnetic properties of high-spin d(6) ions at trigonal prism and linear two-coordinate sites: uniaxial magnetic properties of Ca(3)Co(2)O(6) and Fe[C(SiMe(3))(3)](2). *Inorganic Chemistry*, **2005**, 44, 4407-14	5.1	58
241	Electronic origin of scanning tunneling microscopy images and carbon skeleton orientations of normal alkanes adsorbed on graphite. *Advanced Materials*, **1993**, 5, 817-821	24	58
240	Prediction of Spin Orientations in Terms of HOMO-LUMO Interactions Using Spin-Orbit Coupling as Perturbation. *Accounts of Chemical Research*, **2015**, 48, 3080-7	24.3	56
239	Dimethylammonium copper formate [(CH3)2NH2]Cu(HCOO)3: A metal-organic framework with quasi-one-dimensional antiferromagnetism and magnetostriction. *Physical Review B*, **2013**, 87,	3.3	54
238	Cu(HCO2)2L {L = pyrazine, 4,4?-bipyridine}: employing the formate anion as a building block in three-dimensional coordination polymers. *Dalton Transactions*, **2003**, 2905-2911	4.3	53
237	Organic□norganic hybrid perovskites ABI3 (A = CH3NH3, NH2CHNH2; B = Sn, Pb) as potential thermoelectric materials: a density functional evaluation. *RSC Advances*, **2015**, 5, 78701-78707	3.7	51
236	Interpretation of the magnetic structures of Cu2Te2O5X2 (X = Cl, Br) and Ca3.1Cu0.9RuO6 on the basis of electronic structure considerations: cases for strong super-superexchange interactions involving Cu2+ ions. *Inorganic Chemistry*, **2003**, 42, 3898-906	5.1	50
235	Effect of Viscoelastic Properties of Polymers on the Phase Shift in Tapping Mode Atomic Force Microscopy. *Langmuir*, **1998**, 14, 7343-7347	4	49
234	Selective photocatalytic conversion of alcohol to aldehydes by singlet oxygen over Bi-based metal-organic frameworks under UV□is light irradiation. *Applied Catalysis B: Environmental*, **2019**, 254, 463-470	21.8	46
233	Characterization of the Fermi surface of the organic superconductor - by measurements of Shubnikov-de Haas and angle-dependent magnetoresistance oscillations and by electronic band-structure calculations. *European Physical Journal B*, **1998**, 1, 295-300	1.2	46

232	Importance of the indentation depth in tapping-mode atomic force microscopy study of compliant materials. *Applied Physics Letters*, **1999**, 75, 4198-4200	3.4	46
231	A genuine two-dimensional Ising ferromagnet with magnetically driven re-entrant transition. *Angewandte Chemie - International Edition*, **2012**, 51, 11745-9	16.4	45
230	Prediction for room-temperature half-metallic ferromagnetism in the half-fluorinated single layers of BN and ZnO. *Applied Physics Letters*, **2010**, 97, 122503	3.4	45
229	Electron□Hole Pair Generation of the Visible-Light Plasmonic Photocatalyst [email´protected]: Enhanced Optical Transitions Involving Midgap Defect States of AgCl. *Journal of Physical Chemistry C*, **2014**, 118, 12133-12140	3.8	44
228	Thermodynamically stable single-side hydrogenated graphene. *Physical Review B*, **2010**, 82,	3.3	44
227	Structural and magnetic dimers in the spin-gapped system CuTe2O5. *Physical Review B*, **2006**, 74,	3.3	44
226	Structural Characterization and Band Electronic Structure of □(BEDT-TTF)2I3 below its 135 K Phase Transition. *Molecular Crystals and Liquid Crystals*, **1986**, 138, 393-410		44
225	STM study of molecular order and defects in the layers of cycloalkanes (CH2)48 and (CH2)72 adsorbed on graphite. *Advanced Materials*, **1993**, 5, 821-826	24	42
224	Effect of magnetic dipole-dipole interactions on the spin orientation and magnetic ordering of the spin-ladder compound Sr3Fe2O5. *Inorganic Chemistry*, **2009**, 48, 9051-3	5.1	41
223	Investigations of the oxidation states and spin distributions in Ca3Co2O6 and Ca3CoRhO6 by spin-polarized electronic band structure calculations. *Solid State Communications*, **2003**, 125, 413-417	1.6	41
222	Examination of Butadiene/Styrene-co-butadiene Rubber Blends by Tapping Mode Atomic Force Microscopy. Importance of the Indentation Depth and Reduced Tip□Sample Energy Dissipation in Tapping Mode Atomic Force Microscopy Study of Elastomers. *Langmuir*, **2000**, 16, 5702-5711	4	41
221	The Large Second-Harmonic Generation of LiCs PO is caused by the Metal-Cation-Centered Groups. *Angewandte Chemie - International Edition*, **2018**, 57, 3933-3937	16.4	40
220	Effect of Nonmagnetic Substituents Mg and Zn on the Phase Competition in the Multiferroic Antiferromagnet MnWO4. *Chemistry of Materials*, **2009**, 21, 5203-5214	9.6	40
219	Crystal structure, physical properties and electronic structure of a new organic conductor □-(BEDT-TTF)2SF5CHFCF2SO3. *Journal of Materials Chemistry*, **2001**, 11, 2008-2013		40
218	Lattice dynamical analogies and differences between SrTiO3 and EuTiO3 revealed by phonon-dispersion relations and double-well potentials. *Physical Review B*, **2011**, 84,	3.3	38
217	Investigation of the incommensurate and commensurate magnetic superstructures of LiCuVO4 and CuO on the basis of the isotropic spin exchange and classical spin approximations. *Inorganic Chemistry*, **2004**, 43, 4026-35	5.1	38
216	Spin dimer analysis of the anisotropic spin exchange interactions in the distorted wolframite-type oxides CuWO4, CuMoO4-III, and Cu(Mo(0.25)W0.75)O4. *Inorganic Chemistry*, **2001**, 40, 2161-9	5.1	38
215	Unified model of ferroelectricity induced by spin order. *Physical Review B*, **2013**, 88,	3.3	37

214	Ferrimagnetism in zigzag graphene nanoribbons induced by main-group adatoms. *Applied Physics Letters*, **2010**, 96, 102503	3.4	37
213	Magnetic states of zigzag graphene nanoribbons from first principles. *Applied Physics Letters*, **2009**, 94, 223105	3.4	37
212	Transition-metal anions in solids and their implications on bonding. *Angewandte Chemie - International Edition*, **2006**, 45, 7465-9	16.4	37
211	STRUCTURAL AND ELECTRONIC ORIGIN OF THE HIDDEN NESTING AND CHARGE DENSITY WAVES IN TRANSITION METAL OXIDES AND BRONZES. *International Journal of Modern Physics B*, **1993**, 07, 4005-4043	1.1	36
210	Triple-Kagomé Layer Slabs of Mixed-Valence Rare-Earth Ions Exhibiting Quantum Spin Liquid Behaviors: Synthesis and Characterization of EuMgSBO. *Journal of the American Chemical Society*, **2019**, 141, 9533-9536	16.4	34
209	Consequences of the intrachain dimer-monomer spin frustration and the interchain dimer-monomer spin exchange in the diamond-chain compound azurite Cu(3)(CO(3))(2)(OH)(2). *Journal of Physics Condensed Matter*, **2009**, 21, 392201	1.8	34
208	Analysis of the spin exchange interactions in the three phases of vanadium pyrophosphate, (VO)2P2O7, in terms of spin-orbital interaction energy. *Inorganic Chemistry*, **2000**, 39, 3599-604	5.1	34
207	Importance of the Phthalocyanine Ring Carbon π-orbitals in the Electrical Conduction of Metal Phthalocyanine Polymers. *Israel Journal of Chemistry*, **1983**, 23, 133-138	3.4	34
206	Ultrafast atomic layer-by-layer oxygen vacancy-exchange diffusion in double-perovskite LnBaCo2O5.5+δ thin films. *Scientific Reports*, **2014**, 4, 4726	4.9	33
205	Single-ion anisotropy, Dzyaloshinskii-Moriya interaction, and negative magnetoresistance of the spin-12 pyrochlore R2V2O7. *Physical Review B*, **2011**, 83,	3.3	33
204	Incommensurate spin correlation driven by frustration in BiCu2PO6. *Physical Review B*, **2009**, 80,	3.3	32
203	Magnetic structure and ferroelectric polarization of MnWO4 investigated by density functional calculations and classical spin analysis. *Physical Review B*, **2009**, 80,	3.3	32
202	Insights into How Fluorine-Adsorption and n-Type Doping Affect the Relative Stability of the (001) and (101) Surfaces of TiO2: Enhancing the Exposure of More Active but Thermodynamically Less Stable (001). *Journal of Physical Chemistry Letters*, **2015**, 6, 1876-82	6.4	31
201	Spin dimer analysis of the spin exchange interactions in paramelaconite Cu(4)O(3) and its analogue Ag(2)Cu(2)O(3) and the spin ordering of the Cu(2)O(3) spin lattice leading to their magnetic phase transitions. *Inorganic Chemistry*, **2002**, 41, 3570-7	5.1	30
200	NiII Coordination to an Al-Based Metal–Organic Framework Made from 2-Aminoterephthalate for Photocatalytic Overall Water Splitting. *Angewandte Chemie*, **2017**, 129, 3082-3086	3.6	29
199	An efficient visible-light photocatalyst made from a nonpolar layered semiconductor by grafting electron-withdrawing organic molecules to its surface. *Chemical Communications*, **2016**, 52, 13507-13510	5.8	29
198	Theoretical investigation of the spin exchange interactions and magnetic properties of the homometallic ludwigite Fe(3)O(2)BO(3). *Inorganic Chemistry*, **2002**, 41, 2193-201	5.1	29
197	Structure and Composition of the 200 K-Superconducting Phase of H2 S at Ultrahigh Pressure: The Perovskite (SH(-))(H3 S(+)). *Angewandte Chemie - International Edition*, **2016**, 55, 3682-4	16.4	28

196	On the nature of the spin frustration in the CuO2 ribbon chains of LiCuVO4: crystal structure determination at 1.6 K, magnetic susceptibility analysis, and density functional evaluation of the spin exchange constants. *Inorganic Chemistry*, **2011**, 50, 3582-8	5.1	28
195	Origin of the Ising ferrimagnetism and spin-charge coupling in LuFe2O4. *Physical Review B*, **2009**, 80,	3.3	27
194	Ferromagnetically coupled Shastry-Sutherland quantum spin singlets in (CuCl)LaNb□□ *Physical Review Letters*, **2010**, 105, 167205	7.4	26
193	Improving the photocatalytic hydrogen evolution of UiO-67 by incorporating Ce4+-coordinated bipyridinedicarboxylate ligands. *Science Bulletin*, **2019**, 64, 1502-1509	10.6	25
192	Increasing the Phase-Transition Temperatures in Spin-Frustrated Multiferroic MnWO4 by Mo Doping. *Chemistry of Materials*, **2012**, 24, 353-360	9.6	25
191	Density-functional analysis of spin exchange and ferroelectric polarization in AgCrO2. *Physical Review B*, **2009**, 80,	3.3	25
190	Intense Single Red Emission Induced by Near-Infrared Irradiation Using a Narrow Bandgap Oxide BiVO4 as the Host for Yb3+ and Tm3+ Ions. *Advanced Optical Materials*, **2018**, 6, 1701331	8.1	25
189	Investigation of the spin exchange interactions and the magnetic structure of the high-temperature multiferroic CuBr2. *Physical Review B*, **2012**, 86,	3.3	24
188	Theoretical Investigation of the Magnetic Structure and Ferroelectric Polarization of the Multiferroic Langasite Ba3NbFe3Si2O14. *Chemistry of Materials*, **2010**, 22, 5290-5295	9.6	24
187	Spin-Peierls transition in the S=12 compound TiPO4 featuring large intrachain coupling. *Physical Review B*, **2011**, 83,	3.3	24
186	Spin dimer and classical spin analyses of the ordered magnetic structures of alkali iron pyrophosphates NaFeP(2)O(7) and LiFeP(2)O(7). *Dalton Transactions*, **2004**, 3019-25	4.3	24
185	Oxygen-Vacancy-Induced Midgap States Responsible for the Fluorescence and the Long-Lasting Phosphorescence of the Inverse Spinel Mg(Mg,Sn)O4. *Chemistry of Materials*, **2017**, 29, 1069-1075	9.6	23
184	Seebeck Coefficients of Layered BiCuSeO Phases: Analysis of Their Hole-Density Dependence and Quantum Confinement Effect. *Chemistry of Materials*, **2017**, 29, 2348-2354	9.6	23
183	Orbital order and partial electronic delocalization in a triangular magnetic metal Ag2MnO2. *Physical Review B*, **2010**, 81,	3.3	23
182	Quasi-one-dimensional antiferromagnetism and multiferroicity in CuCrO4. *Physical Review B*, **2011**, 84,	3.3	23
181	Magnetic superstructures of cupric oxide CuO as ordered arrangements of one-dimensional antiferromagnetic chains. *Inorganic Chemistry*, **2003**, 42, 1187-92	5.1	23
180	Magnetic field-temperature phase diagram of multiferroic [(CH3)2NH2]Mn(HCOO)3. *Physical Review B*, **2017**, 96,	3.3	22
179	Strongly correlated one-dimensional magnetic behavior of NiTa2O6. *Physical Review B*, **2014**, 89,	3.3	21

178	Magnetic and electrode properties, structure and phase relations of the layered triangular-lattice tellurate Li4NiTeO6. *Journal of Solid State Chemistry*, **2015**, 225, 89-96	3.3	20
177	Most spin-1/2 transition-metal ions do have single ion anisotropy. *Journal of Chemical Physics*, **2014**, 141, 124113	3.9	20
176	First-principles study of the electronic and magnetic structures of the tetragonal and orthorhombic phases of Ca3Mn2O7. *Physical Review B*, **2007**, 76,	3.3	20
175	A two-dimensional radical salt based upon BEDT-TTF and the dimeric, magnetic anion [Fe(tdas)2]22□(BEDT-TTF)2[Fe(tdas)2](tdas = 1,2,5-thiadiazole-3,4-dithiolate). *Journal of Materials Chemistry*, **2002**, 12, 3570-3577		20
174	Electronic and Structural Factors Controlling the Spin Orientations of Magnetic Ions. *Inorganic Chemistry*, **2019**, 58, 11854-11874	5.1	19
173	Loss of Linear Band Dispersion and Trigonal Structure in Silicene on Ir(111). *Journal of Physical Chemistry Letters*, **2015**, 6, 1065-70	6.4	19
172	Strong single-ion anisotropy and anisotropic interactions of magnetic adatoms induced by topological surface states. *Physical Review B*, **2012**, 85,	3.3	19
171	Density functional theory analysis of the interplay between Jahn-Teller instability, uniaxial magnetism, spin arrangement, metal-metal interaction, and spin-orbit coupling in Ca3CoMO6 (M = Co, Rh, Ir). *Inorganic Chemistry*, **2011**, 50, 1758-66	5.1	19
170	A Magnetic Transition Probed by the Ce Ion in Square-Lattice Antiferromagnet CeMnAsO. *Journal of the Physical Society of Japan*, **2011**, 80, 094708	1.5	19
169	On the Conflicting Pictures of Magnetism for the Frustrated Triangular Lattice Antiferromagnet CuFeO2. *Chemistry of Materials*, **2006**, 18, 1268-1274	9.6	19
168	Electron Counting Scheme Relevant for Late Transition Metal Compounds with Weakly Electronegative Ligands. Electronic Band Structure Study of Phosphosilicides PtSi3P2 and NiSi2P3□ *Inorganic Chemistry*, **1999**, 38, 340-345	5.1	19
167	Enhancing the Photoelectrochemical Water Oxidation Reaction of BiVO4 Photoanode by Employing Carbon Spheres as Electron Reservoirs. *ACS Catalysis*, **2020**, 10, 13031-13039	13.1	18
166	Quantum critical transition amplifies magnetoelastic coupling in Mn[N(CN)2]2. *Physical Review Letters*, **2013**, 110, 237202	7.4	17
165	Metal Anions in Metal-Rich Compounds and Polar Intermetallics. *European Journal of Inorganic Chemistry*, **2011**, 2011, 3841-3847	2.3	17
164	One-Dimensional Semiconducting Chains of the Quaternary Zintl Anion in (Et4N)4[Au(Ag1-xAux)2Te9]. *Angewandte Chemie International Edition in English*, **1997**, 36, 1087-1090		17
163	Effect of metal-ligand bond lengths on superexchange interactions in Jahn-Teller d(4) ion systems: spin dimer analysis of the magnetic structure of marokite CaMn(2)O(4). *Inorganic Chemistry*, **2002**, 41, 5575-81	5.1	17
162	Perspective on □An extended H□kel theory. I. Hydrocarbons□*Theoretical Chemistry Accounts*, **2000**, 103, 252-256	1.9	17
161	Description of ligand field splitting in terms of density functional theory: Calculations of the split levels of the 2F5/2 and 2F7/2 subterms in CeO and CeF under the weak field coupling scheme. *Journal of Chemical Physics*, **1998**, 108, 3479-3488	3.9	17

160	Catalytic Dynamics and Oxygen Diffusion in Doped PrBaCo2O(5.5+)Thin Films. *ACS Applied Materials & Interfaces*, **2015**, 7, 24353-9	9.5	16
159	Spin reorientation in the square-lattice antiferromagnets RMnAsO (R = Ce, Nd): density functional analysis of the spin-exchange interactions between the rare-earth and transition-metal ions. *Inorganic Chemistry*, **2012**, 51, 6890-7	5.1	16
158	Magneto-optical properties and charge-spin coupling in the molecular (2,3-dmpyH)2CuBr4 spin-ladder material. *Physical Review B*, **2010**, 81,	3.3	16
157	The Large Second-Harmonic Generation of LiCs2PO4 is caused by the Metal-Cation-Centered Groups. *Angewandte Chemie*, **2018**, 130, 3997-4001	3.6	15
156	Magneto-Optical Kerr Switching Properties of (CrI3)2 and (CrBr3/CrI3) Bilayers. *ACS Applied Electronic Materials*, **2020**, 2, 1373-1380	4	14
155	Endotaxial Growth of [100]-Oriented TaON Films on LiTaO3 Single Crystals for Enhanced Photoelectrochemical Water Splitting. *Solar Rrl*, **2018**, 2, 1700243	7.1	14
154	Characterization of the spin-12 linear-chain ferromagnet CuAs2O4. *Physical Review B*, **2014**, 89,	3.3	14
153	The Road Map toward Room-Temperature Superconductivity: Manipulating Different Pairing Channels in Systems Composed of Multiple Electronic Components. *Condensed Matter*, **2017**, 2, 24	1.8	14
152	Spin orientations of the spin-half Ir(4+) ions in Sr3NiIrO6, Sr2IrO4, and Na2IrO3: Density functional, perturbation theory, and Madelung potential analyses. *Journal of Chemical Physics*, **2016**, 144, 114706	3.9	14
151	Spin-Peierls distortions in TiPO4. *Physical Review B*, **2013**, 88,	3.3	13
150	The layered ferromagnet Cs2AgF4: Antiferromagnetic inter-layer coupling driven by magnetic dipole-dipole interactions. *Zeitschrift F Kristallographie*, **2010**, 225,		13
149	Site preference of Eu2+ dopants in the (Ba,Sr)13Al22xSi10+2xO66 phosphor and its effect on the luminescence properties: a density functional investigation. *Journal of Materials Chemistry*, **2009**, 19, 9170		13
148	Atomically layer-by-layer diffusion of oxygen/hydrogen in highly epitaxial PrBaCo2O5.5+thin films. *Applied Physics Letters*, **2015**, 107, 243903	3.4	12
147	Enhancing the Efficiency of Water Oxidation by Boron-Doped BiVO under Visible Light: Hole Trapping by BO Tetrahedra. *ChemPlusChem*, **2015**, 80, 1113-1118	2.8	12
146	Tolerance Factor and CationAnion Orbital Interactions Differentiating the Polar and Antiferrodistortive Structures of Perovskite Oxides ABO3. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2015**, 641, 1043-1052	1.3	12
145	On the Strength of the C?HD Hydrogen Bond and the Eclipsed Arrangement of the Methyl Group in a Tricyclic Orthoamide Trihydrate. *Angewandte Chemie International Edition in English*, **1993**, 32, 588-589		12
144	Aurivillius Phases: A Possible New Class of Metal Oxide Superconductors. *Angewandte Chemie International Edition in English*, **1989**, 28, 750-751		12
143	The Orbital Interaction Approach to Structural and Conformational Problems in Organic Chemistry. *Israel Journal of Chemistry*, **1980**, 20, 36-42	3.4	12

142	Structural and Magnetic Properties of the Trirutile-type 1D-Heisenberg Anti-Ferromagnet CuTaO. *Inorganic Chemistry*, **2017**, 56, 6318-6329	5.1	11
141	AMnXO Family (A = Li, Na, Ag; X = Si, Ge): Structural and Magnetic Properties. *Inorganic Chemistry*, **2017**, 56, 14023-14039	5.1	11
140	On Why the Two Polymorphs of NaFePO4 Exhibit Widely Different Magnetic Structures: Density Functional Analysis. *Inorganic Chemistry*, **2015**, 54, 4966-71	5.1	11
139	Molybdenum Nitride Electrocatalysts for Hydrogen Evolution More Efficient than Platinum/Carbon: MoN/CeO@Nickel Foam. *ACS Applied Materials & Interfaces*, **2020**, 12, 29153-29161	9.5	11
138	A Genuine Two-Dimensional Ising Ferromagnet with Magnetically Driven Re-entrant Transition. *Angewandte Chemie*, **2012**, 124, 11915-11919	3.6	11
137	Description of Anhydrous (Black) Dioptase as a S = 1/2 Uniform Antiferromagnetic Chain System´. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2010**, 636, 54-61	1.3	11
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