Bo Brummerstedt Iversen

List of Publications by Citations

520 papers	18,151 citations	67 h-index	106 g-index
577 ext. papers	20,192 ext. citations	6.3 avg, IF	6.95 L-index

#	Paper	IF	Citations
520	Disordered zinc in Zn4Sb3 with phonon-glass and electron-crystal thermoelectric properties. *Nature Materials*, **2004**, 3, 458-63	27	690
519	Avoided crossing of rattler modes in thermoelectric materials. *Nature Materials*, **2008**, 7, 811-5	27	452
518	Coexistence of the topological state and a two-dimensional electron gas on the surface of Bi(2)Se(3). *Nature Communications*, **2010**, 1, 128	17.4	361
517	Large tunable Rashba spin splitting of a two-dimensional electron gas in Bi2Se3. *Physical Review Letters*, **2011**, 107, 096802	7.4	351
516	Discovery of high-performance low-cost n-type MgSb-based thermoelectric materials with multi-valley conduction bands. *Nature Communications*, **2017**, 8, 13901	17.4	297
515	Thermoelectric clathrates of type I. *Dalton Transactions*, **2010**, 39, 978-92	4.3	245
514	Three new co-crystals of hydroquinone: crystal structures and Hirshfeld surface analysis of intermolecular interactions. *New Journal of Chemistry*, **2010**, 34, 193-199	3.6	236
513	Measuring thermoelectric transport properties of materials. *Energy and Environmental Science*, **2015**, 8, 423-435	35.4	210
512	Colossal Seebeck coefficient in strongly correlated semiconductor FeSb 2. *Europhysics Letters*, **2007** , 80, 17008	1.6	195
511	Measurement of the electrical resistivity and Hall coefficient at high temperatures. *Review of Scientific Instruments*, **2012**, 83, 123902	1.7	186
510	Designing high-performance layered thermoelectric materials through orbital engineering. *Nature Communications*, **2016**, 7, 10892	17.4	165
509	Elucidating Negative Thermal Expansion in MOF-5. *Journal of Physical Chemistry C*, **2010**, 114, 16181-16186	3.6	157
508	Thermal conductivity of thermoelectric clathrates. *Physical Review B*, **2004**, 69,	3.3	155
507	Interstitial Zn atoms do the trick in thermoelectric zinc antimonide, Zn4Sb3: a combined maximum entropy method X-ray electron density and ab initio electronic structure study. *Chemistry - A European Journal*, **2004**, 10, 3861-70	4.8	151
506	Revealing the mechanisms behind SnO2 nanoparticle formation and growth during hydrothermal synthesis: an in situ total scattering study. *Journal of the American Chemical Society*, **2012**, 134, 6785-92	16.4	150
505	Crystal structures of thermoelectric n- and p-type Ba8Ga16Ge30 studied by single crystal, multitemperature, neutron diffraction, conventional X-ray diffraction and resonant synchrotron X-ray diffraction. *Journal of the American Chemical Society*, **2006**, 128, 15657-65	16.4	147
504	Quantitative analysis of intermolecular interactions in orthorhombic rubrene. *IUCrJ*, **2015**, 2, 563-74	4.7	145

503	Topological Analysis of the Charge Density in Short Intramolecular O□H□□O Hydrogen Bonds. Very Low Temperature X-ray and Neutron Diffraction Study of Benzoylacetone. *Journal of the American Chemical Society*, **1998**, 120, 10040-10045	16.4	136
502	In-plane magnetic anisotropy of Fe atoms on Bi2Se3(111). *Physical Review Letters*, **2012**, 108, 256811	7.4	133
501	High temperature thermoelectric efficiency in Ba8Ga16Ge30. *Physical Review B*, **2008**, 77,	3.3	129
500	Crystal structures, atomic vibration, and disorder of the type-I thermoelectric clathrates Ba8Ga16Si30, Ba8Ga16Ge30, Ba8In16Ge30, and Sr8Ga16Ge30. *Physical Review B*, **2005**, 71,	3.3	127
499	Simultaneous quantization of bulk conduction and valence states through adsorption of nonmagnetic impurities on Bi2Se3. *Physical Review Letters*, **2011**, 107, 086802	7.4	125
498	On the electronic nature of low-barrier hydrogen bonds in enzymatic reactions. *Proceedings of the National Academy of Sciences of the United States of America*, **1998**, 95, 12799-802	11.5	120
497	Why are Clathrates Good Candidates for Thermoelectric Materials?. *Journal of Solid State Chemistry*, **2000**, 149, 455-458	3.3	117
496	Enhanced Thermoelectric Performance through Tuning Bonding Energy in Cu2Se1−xSx Liquid-like Materials. *Chemistry of Materials*, **2017**, 29, 6367-6377	9.6	115
495	Characterization of the Short Strong Hydrogen Bond in Benzoylacetone by ab Initio Calculations and Accurate Diffraction Experiments. Implications for the Electronic Nature of Low-Barrier Hydrogen Bonds in Enzymatic Reactions. *Journal of the American Chemical Society*, **1998**, 120, 12117-12124	16.4	115
494	Experimental setup forin situX-ray SAXS/WAXS/PDF studies of the formation and growth of nanoparticles in near- and supercritical fluids. *Journal of Applied Crystallography*, **2010**, 43, 729-736	3.8	109
493	High-Performance Low-Cost n-Type Se-Doped Mg3Sb2-Based Zintl Compounds for Thermoelectric Application. *Chemistry of Materials*, **2017**, 29, 5371-5383	9.6	108
492	Solvothermal synthesis of new metal organic framework structures in the zinc□erephthalic acid□imethyl formamide system. *Journal of Solid State Chemistry*, **2005**, 178, 3342-3351	3.3	107
491	Effect of hydrothermal liquefaction aqueous phase recycling on bio-crude yields and composition. *Bioresource Technology*, **2016**, 220, 190-199	11	103
490	In situ studies of solvothermal synthesis of energy materials. *ChemSusChem*, **2014**, 7, 1594-611	8.3	101
489	Ultrahigh thermoelectric performance in Cu 2□ Se 0.5 S 0.5 liquid-like materials. *Materials Today Physics*, **2017**, 1, 14-23	8	99
488	Evidence for a direct band gap in the topological insulator Bi2Se3 from theory and experiment. *Physical Review B*, **2013**, 87,	3.3	96
487	Stability of the Bi2Se3(111) topological state: Electron-phonon and electron-defect scattering. *Physical Review B*, **2011**, 83,	3.3	93
486	The influence of crystallite size and crystallinity of anatase nanoparticles on the photo-degradation of phenol. *Journal of Catalysis*, **2014**, 310, 100-108	7.3	91

485	Phase transition enhanced thermoelectric figure-of-merit in copper chalcogenides. *APL Materials*, **2013**, 1, 052107	5.7	91
484	Controllable magnetic doping of the surface state of a topological insulator. *Physical Review Letters* , **2013**, 110, 126804	7.4	90
483	Host Structure Engineering in Thermoelectric Clathrates. *Chemistry of Materials*, **2007**, 19, 4896-4905	9.6	90
482	Location of Cu(2+) in CHA zeolite investigated by X-ray diffraction using the Rietveld/maximum entropy method. *IUCrJ*, **2014**, 1, 382-6	4.7	90
481	First experimental characterization of a non-nuclear attractor in a dimeric magnesium(I) compound. *Journal of Physical Chemistry A*, **2011**, 115, 194-200	2.8	88
480	Testing the concept of hypervalency: charge density analysis of K2SO4. *Inorganic Chemistry*, **2012**, 51, 8607-16	5.1	87
479	Biomolecule-assisted hydrothermal synthesis and self-assembly of Bi2Te3 nanostring-cluster hierarchical structure. *ACS Nano*, **2010**, 4, 2523-30	16.7	86
478	Experimental and theoretical charge density studies at subatomic resolution. *Journal of Physical Chemistry A*, **2011**, 115, 13061-71	2.8	84
477	Experimental and theoretical investigations of strongly correlated FeSb2−xSnx. *Physical Review B*, **2006**, 74,	3.3	84
476	Modeling the thermal conductivities of the zinc antimonides ZnSb and Zn4Sb3. *Physical Review B*, **2014**, 89,	3.3	83
475	Direct Evidence of Cation Disorder in Thermoelectric Lead Chalcogenides PbTe and PbS. *Advanced Functional Materials*, **2013**, 23, 5477-5483	15.6	83
474	Simultaneous improvement of power factor and thermal conductivity via Ag doping in p-type Mg3Sb2 thermoelectric materials. *Journal of Materials Chemistry A*, **2017**, 5, 4932-4939	13	79
473	Understanding the formation and evolution of ceria nanoparticles under hydrothermal conditions. *Angewandte Chemie - International Edition*, **2012**, 51, 9030-3	16.4	78
472	Low-Temperature Structural Transitions in the Phonon-Glass Thermoelectric Material Zn4Sb3: Ordering of Zn Interstitials and Defects. *Chemistry of Materials*, **2007**, 19, 834-838	9.6	77
471	Experimental evidence for the existence of non-nuclear maxima in the electron-density distribution of metallic beryllium. A comparative study of the maximum entropy method and the multipole refinement method. *Acta Crystallographica Section B: Structural Science*, **1995**, 51 (Pt 4), 580-91		77
470	Ab initio Calculations of Intrinsic Point Defects in ZnSb. *Chemistry of Materials*, **2012**, 24, 2111-2116	9.6	75
469	Defects in Hydrothermally Synthesized LiFePO4 and LiFe1-xMnxPO4 Cathode Materials. *Chemistry of Materials*, **2013**, 25, 2282-2290	9.6	75
468	Time-resolved in situ synchrotron X-ray study and large-scale production of magnetite nanoparticles in supercritical water. *Angewandte Chemie - International Edition*, **2009**, 48, 4788-91	16.4	75

467	Critical size of crystalline ZrO(2) nanoparticles synthesized in near- and supercritical water and supercritical isopropyl alcohol. *ACS Nano*, **2008**, 2, 1058-68	16.7	75
466	Synthesis, physical properties, multitemperature crystal structure, and 20 K synchrotron X-ray charge density of a magnetic metal organic framework structure, Mn3(C8O4H4)3(C5H11ON)2. *Journal of the American Chemical Society*, **2005**, 127, 9156-66	16.4	75
465	Interrelation between atomic switching disorder and thermoelectric properties of ZrNiSn half-Heusler compounds. *CrystEngComm*, **2012**, 14, 4467	3.3	74
464	Narrow band gap and enhanced thermoelectricity in FeSb2. *Dalton Transactions*, **2010**, 39, 1012-9	4.3	72
463	Enhanced Thermoelectric Properties in Zinc Antimonides. *Chemistry of Materials*, **2011**, 23, 3907-3914	9.6	71
462	Experimental and theoretical charge density study of chemical bonding in a Co dimer complex. *Journal of the American Chemical Society*, **2008**, 130, 3834-43	16.4	71
461	Electronic structure and transport in the low-temperature thermoelectric CsBi4Te6: Semiclassical transport equations. *Physical Review B*, **2006**, 73,	3.3	71
460	Supercritical Propanol□Water Synthesis and Comprehensive Size Characterisation of Highly Crystalline anatase TiO2 Nanoparticles. *Journal of Solid State Chemistry*, **2006**, 179, 2674-2680	3.3	71
459	Multi-Temperature Crystallographic Studies of Mixed-Valence Polynuclear Complexes; Valence Trapping Process in the Trinuclear Oxo-Bridged Iron Compound, [Fe3O(O2CC(CH3)3)6(C5H5N)3]. *Journal of the American Chemical Society*, **2000**, 122, 11370-11379	16.4	71
458	Anisotropic Crystal Growth Kinetics of Anatase TiO2 Nanoparticles Synthesized in a Nonaqueous Medium. *Chemistry of Materials*, **2010**, 22, 6044-6055	9.6	69
457	Nanostructured Co1□Nix(Sb1□Tey)3 skutterudites: Theoretical modeling, synthesis and thermoelectric properties. *Journal of Applied Physics*, **2005**, 97, 044317	2.5	68
456	The charge density distribution in a model compound of the catalytic triad in serine proteases. *Chemistry - A European Journal*, **2001**, 7, 3756-67	4.8	68
455	Direct Growth of Highly Strained Pt Islands on Branched Ni Nanoparticles for Improved Hydrogen Evolution Reaction Activity. *Journal of the American Chemical Society*, **2019**, 141, 16202-16207	16.4	67
454	In situ high-energy synchrotron radiation study of sol-gel nanoparticle formation in supercritical fluids. *Angewandte Chemie - International Edition*, **2007**, 46, 1113-6	16.4	67
453	Hg0.04Zn3.96Sb3: Synthesis, Crystal Structure, Phase Transition, and Thermoelectric Properties. *Chemistry of Materials*, **2007**, 19, 6304-6311	9.6	67
452	Large Seebeck effect by charge-mobility engineering. *Nature Communications*, **2015**, 6, 7475	17.4	66
451	The chemistry of nucleation. *CrystEngComm*, **2016**, 18, 8332-8353	3.3	65
450	Mechanisms for iron oxide formation under hydrothermal conditions: an in situ total scattering study. *ACS Nano*, **2014**, 8, 10704-14	16.7	65

449	Crystal Structure, Band Structure, and Physical Properties of Ba8Cu6-xGe40+x(0 ⊠0.7). *Chemistry of Materials*, **2006**, 18, 4633-4642	9.6	64
448	Guest-framework interaction in type I inorganic clathrates with promising thermoelectric properties: on the ionic versus neutral nature of the alkaline-earth metal guest A in A8Ga16Ge30 (A=Sr, Ba). *Chemistry - A European Journal*, **2003**, 9, 4556-68	4.8	64
447	Improvements and considerations for size distribution retrieval from small-angle scattering data by Monte Carlo methods. *Journal of Applied Crystallography*, **2013**, 46, 365-371	3.8	63
446	FeSb2: Prototype of huge electron-diffusion thermoelectricity. *Physical Review B*, **2009**, 79,	3.3	63
445	Redox-Driven Migration of Copper Ions in the Cu-CHA Zeolite as Shown by the In Situ PXRD/XANES Technique. *Angewandte Chemie - International Edition*, **2017**, 56, 10367-10372	16.4	62
444	Maximum entropy method analysis of thermal motion and disorder in thermoelectric clathrate Ba8Ga16Si30. *Journal of Applied Physics*, **2002**, 91, 5694-5699	2.5	62
443	Synthesis and characterization of basic bismuth(III) nitrates. *Dalton Transactions RSC*, **2000**, 265-270		62
442	X-ray electron density investigation of chemical bonding in van der Waals materials. *Nature Materials*, **2018**, 17, 249-252	27	61
441	Surface-dominated transport on a bulk topological insulator. *Nano Letters*, **2014**, 14, 3755-60	11.5	61
440	Thermally stable thermoelectric Zn4Sb3 by zone-melting synthesis. *Applied Physics Letters*, **2008**, 92, 161907	3.4	61
439	Cu8GeSe6-based thermoelectric materials with an argyrodite structure. *Journal of Materials Chemistry C*, **2017**, 5, 943-952	7.1	60
438	Probing the accuracy and precision of Hirshfeld atom refinement with interfaced with. *IUCrJ*, **2018**, 5, 32-44	4.7	60
437	Electron density distributions of redox active mixed valence carboxylate bridged trinuclear iron complexes. *Journal of the American Chemical Society*, **2003**, 125, 11088-99	16.4	60
436	Huge Thermoelectric Power Factor: FeSb2versus FeAs2and RuSb2. *Applied Physics Express*, **2009**, 2, 091102	2.4	59
435	Metastable formation of low temperature cubic Li2TiO3 under hydrothermal conditions Its stability and structural properties. *Solid State Ionics*, **2010**, 181, 1525-1529	3.3	58
434	Nonstoichiometry and chemical purity effects in thermoelectric Ba8Ga16Ge30 clathrate. *Journal of Applied Physics*, **2002**, 92, 7281-7290	2.5	58
433	General Solvothermal Synthesis Method for Complete Solubility Range Bimetallic and High-Entropy Alloy Nanocatalysts. *Advanced Functional Materials*, **2019**, 29, 1905933	15.6	57
432	Fulfilling thermoelectric promises: Zn4Sb3 from materials research to power generation. *Journal of Materials Chemistry*, **2010**, 20, 10778		57

431	Strong N-H???O Hydrogen Bonding in a Model Compound of the Catalytic Triad in Serine Proteases. *Angewandte Chemie - International Edition*, **1999**, 38, 1239-1242	16.4	57
430	New Insight on Tuning Electrical Transport Properties via Chalcogen Doping in n-type Mg3Sb2-Based Thermoelectric Materials. *Advanced Energy Materials*, **2018**, 8, 1702776	21.8	56
429	Extremely low thermal conductivity and high thermoelectric performance in liquid-like Cu2Se1−xSx polymorphic materials. *Journal of Materials Chemistry A*, **2017**, 5, 18148-18156	13	56
428	Development and Application of Chemical Analysis Methods for Investigation of Bio-Oils and Aqueous Phase from Hydrothermal Liquefaction of Biomass. *Energy & Fuels*, **2012**, 26, 6988-6998	4.1	55
427	Strong phonon charge carrier coupling in thermoelectric clathrates. *Physical Review B*, **2006**, 73,	3.3	55
426	Host-guest chemistry of the chromium-wheel complex [Cr8F8(tBuCO2)16]: prediction of inclusion capabilities by using an electrostatic potential distribution determined by modeling synchrotron X-ray structure factors at 16 K. *Chemistry - A European Journal*, **2002**, 8, 2775-86	4.8	55
425	The use of synchrotron radiation in X-ray charge density analysis of coordination complexes. *Coordination Chemistry Reviews*, **2005**, 249, 179-195	23.2	55
424	Interanionic O-H small middle dot small middle dot small middle dotO Interactions: The Charge Density Point of View The Oak Ridge National Laboratory is managed by Lockheed Martin Energy Research Corporation for the US Department of Energy (DE-AC05-96OR22464). Prof. M. Moret and Dr. L. Carlucci are thanked for help in crystallizing large samples suitable for the neutron study.	16.4	55
423	Low-cost high-performance zinc antimonide thin films for thermoelectric applications. *Advanced Materials*, **2012**, 24, 1693-6 *Angewandte Chemie - International Edition*, **2000**, 39, 2719-2722	24	54
422	Robust surface doping of Bi2Se3 by rubidium intercalation. *ACS Nano*, **2012**, 6, 7009-15	16.7	54
421	Size and Morphology Dependence of ZnO Nanoparticles Synthesized by a Fast Continuous Flow Hydrothermal Method. *Crystal Growth and Design*, **2011**, 11, 4027-4033	3.5	54
420	Thermoelectric properties of thin films of bismuth telluride electrochemically deposited on stainless steel substrates. *Electrochimica Acta*, **2011**, 56, 4216-4223	6.7	54
419	F center in sodium electrosodalite as a physical manifestation of a non-nuclear attractor in the electron density. *Physical Review B*, **1999**, 59, 12359-12369	3.3	54
418	Chemical bonding origin of the unexpected isotropic physical properties in thermoelectric MgSb and related materials. *Nature Communications*, **2018**, 9, 4716	17.4	54
417	Atomic properties and chemical bonding in the pyrite and marcasite polymorphs of FeS2: a combined experimental and theoretical electron density study. *Chemical Science*, **2014**, 5, 1408-1421	9.4	53
416	In-Situ Synchrotron Radiation Study of Formation and Growth of Crystalline CexZr1−xO2 Nanoparticles Synthesized in Supercritical Water. *Chemistry of Materials*, **2010**, 22, 1814-1820	9.6	53
415	Insights into the design of thermoelectric Mg3Sb2 and its analogs by combining theory and experiment. *Npj Computational Materials*, **2019**, 5,	10.9	52
414	In situ total X-ray scattering study of WO nanoparticle formation under hydrothermal conditions. *Angewandte Chemie - International Edition*, **2014**, 53, 3667-70	16.4	52

413	Controlling Size, Crystallinity, and Electrochemical Performance of Li4Ti5O12 Nanocrystals. *Chemistry of Materials*, **2013**, 25, 5023-5030	9.6	52
412	Experimental electron density study of the Mg-Mg bonding character in a magnesium(I) dimer. *Journal of the American Chemical Society*, **2009**, 131, 4208-9	16.4	52
411	Crystal structure and transport properties of nickel containing germanium clathrates. *Physical Review B*, **2007**, 76,	3.3	52
410	Crystal structure and phase transition of thermoelectric SnSe. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2016**, 72, 310-6	1.8	52
409	Enhanced thermoelectric properties of Mg2Si by addition of TiO2 nanoparticles. *Journal of Applied Physics*, **2012**, 111, 023701	2.5	51
408	Solid State Formation Mechanism of Li4Ti5O12 from an Anatase TiO2 Source. *Chemistry of Materials*, **2014**, 26, 3679-3686	9.6	50
407	In situ X-ray diffraction study of the formation, growth, and phase transition of colloidal Cu(2-x)S nanocrystals. *ACS Nano*, **2014**, 8, 4295-303	16.7	50
406	Optimized carbonation of magnesium silicate mineral for CO2 storage. *ACS Applied Materials & Interfaces*, **2015**, 7, 5258-64	9.5	50
405	Scrutinizing negative thermal expansion in MOF-5 by scattering techniques and ab initio calculations. *Dalton Transactions*, **2013**, 42, 1996-2007	4.3	49
404	Cd Substitution in MxZn4□xSb3: Effect on Thermal Stability, Crystal Structure, Phase Transitions, and Thermoelectric Performance. *Chemistry of Materials*, **2010**, 22, 2375-2383	9.6	49
403	Experimental Charge Densities of Semiconducting Cage Structures Containing Alkaline Earth Guest Atoms Work at the X10c beamline at NSLS was supported by the Division of Materials Sciences of the US Department of Energy (DE-AC02-98CH10886). B.B.I. and A.E.C.P. gratefully acknowledge support from the Danish and Swedish Research Councils (SNF, TFR, STINT). This work was partially	16.4	49
402	ZnO nanoparticle based highly efficient CdS/CdSe quantum dot-sensitized solar cells. *Physical Chemistry Chemical Physics*, **2013**, 15, 8710-5	3.6	48
401	High-Pressure, High-Temperature Formation of Phase-Pure Monoclinic Zirconia Nanocrystals Studied by Time-Resolved in situ Synchrotron X-Ray Diffraction. *Advanced Materials*, **2009**, 21, 3572-3575	24	47
400	Accurate charge densities in days - use of synchrotrons, image plates and very low temperatures. *Acta Crystallographica Section B: Structural Science*, **1999**, 55, 363-374		47
399	Reactor design for in situ X-ray scattering studies of nanoparticle formation in supercritical water syntheses. *Journal of Supercritical Fluids*, **2008**, 44, 385-390	4.2	46
398	Thermoelectric properties of Cu2Se1□Tex solid solutions. *Journal of Materials Chemistry A*, **2018**, 6, 6977-6986	13	45
397	Hydrothermal Liquefaction of the Microalgae Phaeodactylum tricornutum: Impact of Reaction Conditions on Product and Elemental Distribution. *Energy & Fuels*, **2014**, 28, 5792-5803	4.1	45
396	Visualizing lithium-ion migration pathways in battery materials. *Chemistry - A European Journal*, **2013**, 19, 15535-44	4.8	45

395	Hydrothermal co-liquefaction of biomasses quantitative analysis of bio-crude and aqueous phase composition. *Sustainable Energy and Fuels*, **2017**, 1, 789-805	5.8	44
394	Crystal structure across the to phase transition in thermoelectric Cu Se. *IUCrJ*, **2017**, 4, 476-485	4.7	44
393	High thermoelectric performance and low thermal conductivity in Cu2yS1/3Se1/3Te1/3 liquid-like materials with nanoscale mosaic structures. *Nano Energy*, **2017**, 42, 43-50	17.1	44
392	Experimental determination of core electron deformation in diamond. *Acta Crystallographica Section A: Foundations and Advances*, **2014**, 70, 39-48	1.7	44
391	In Situ Powder Diffraction Study of the Hydrothermal Synthesis of ZnO Nanoparticles. *Crystal Growth and Design*, **2014**, 14, 2803-2810	3.5	44
390	High-Temperature and High-Pressure Aqueous Solution Formation, Growth, Crystal Structure, and Magnetic Properties of BiFeO3Nanocrystals. *Chemistry of Materials*, **2011**, 23, 1158-1165	9.6	44
389	Effects of the order disorder phase transition on the physical properties of A8Sn44?2 (A = Rb, Cs). *Journal of Materials Chemistry*, **2008**, 18, 5630		44
388	Are type-I clathrates Zintl phases and phonon glasses and electron single crystals. *Physica B: Condensed Matter*, **2003**, 328, 39-43	2.8	43
387	XN study of the electron density in (ND4)2Cu(SO4)2.6D2O at 9 K: flexible radial functions are vital. *Acta Crystallographica Section B: Structural Science*, **1993**, 49, 794-806		43
386	A P2-NaxCo0.7Mn0.3O2 (x 1.0) cathode material for Na-ion batteries with superior rate and cycle capability. *Journal of Materials Chemistry A*, **2016**, 4, 12281-12288	13	43
385	The electronic structure of clean and adsorbate-covered Bi2Se3: an angle-resolved photoemission study. *Semiconductor Science and Technology*, **2012**, 27, 124001	1.8	42
384	Multitemperature crystal structures and physical properties of the partially filled thermoelectric skutterudites M0.1Co4Sb12(M=La,Ce,Nd,Sm,Yb,andEu). *Physical Review B*, **2011**, 84,	3.3	42
383	Rapid Green Continuous Flow Supercritical Synthesis of High Performance Li4Ti5O12Nanocrystals for Li Ion Battery Applications. *Journal of the Electrochemical Society*, **2011**, 159, A166-A171	3.9	42
382	Experimental and Theoretical Electron Density Study of the Peroxo Function in Oxoperoxo(pyridine-2,6-dicarboxylato)(hexamethylphosphoramide)molybdenum(VI): Implications for Olefin Epoxidation by Peroxo Transition Metal Complexes. *Journal of Physical Chemistry A*, **2001** , 105, 9234-9242	2.8	42
381	Mechanistic Insight into the Interaction Between a Titanium Dioxide Photocatalyst and Pd Cocatalyst for Improved Photocatalytic Performance. *ACS Catalysis*, **2016**, 6, 4239-4247	13.1	41
380	Effects of heterogeneous catalyst in hydrothermal liquefaction of dried distillers grains with solubles. *Fuel*, **2014**, 123, 158-166	7.1	41
379	Demonstration of thin film pair distribution function analysis (tfPDF) for the study of local structure in amorphous and crystalline thin films. *IUCrJ*, **2015**, 2, 481-9	4.7	41
378	Predicting the Chemical Composition of Aqueous Phase from Hydrothermal Liquefaction of Model Compounds and Biomasses. *Energy & Fuels*, **2016**, 30, 10470-10483	4.1	40

377	Rapid Hydrothermal Preparation of Rutile TiO2 Nanoparticles by Simultaneous Transformation of Primary Brookite and Anatase: An in Situ Synchrotron PXRD Study. *Crystal Growth and Design*, **2012**, 12, 6092-6097	3.5	40
376	Synthesis, crystal structure, atomic Hirshfeld surfaces, and physical properties of hexagonal CeMnNi4. *Inorganic Chemistry*, **2010**, 49, 9343-9	5.1	40
375	Interfacial superconductivity in a bi-collinear antiferromagnetically ordered FeTe monolayer on a topological insulator. *Nature Communications*, **2017**, 8, 14074	17.4	39
374	Evolution of atomic structure during nanoparticle formation. *IUCrJ*, **2014**, 1, 165-71	4.7	39
373	Phase separation and bulk p-n transition in single crystals of Bi□Te□Se topological insulator. *Advanced Materials*, **2013**, 25, 889-93	24	39
372	In situ total X-ray scattering study of the formation mechanism and structural defects in anatase TiO2 nanoparticles under hydrothermal conditions. *CrystEngComm*, **2015**, 17, 6868-6877	3.3	38
371	Coupling in situ synchrotron radiation with ex situ spectroscopy characterizations to study the formation of Ba1□SrxTiO3 nanoparticles in supercritical fluids. *Journal of Supercritical Fluids*, **2014**, 87, 111-117	4.2	38
370	Influence of sample compaction on the thermoelectric performance of Zn4Sb3. *Applied Physics Letters*, **2006**, 89, 242108	3.4	38
369	Formation Mechanisms of Nanocrystalline MnO2 Polymorphs under Hydrothermal Conditions. *Crystal Growth and Design*, **2018**, 18, 827-838	3.5	37
368	Synchrotron X-ray charge density study of coordination polymer Co3(C8H4O4)4(C4H12N)2(C5H11NO)3 at 16 K. *Journal of the American Chemical Society*, **2008**, 130, 7988-96	16.4	37
367	Construction and Commissioning of a Continuous Reactor for Hydrothermal Liquefaction. *Industrial & Engineering Chemistry Research*, **2015**, 54, 5935-5947	3.9	36
366	Role of vacancies in the high-temperature pseudodisplacive phase transition in GeTe. *Physical Review B*, **2018**, 97,	3.3	36
365	Surface structure of Bi2Se3(111) determined by low-energy electron diffraction and surface x-ray diffraction. *Physical Review B*, **2013**, 88,	3.3	36
364	Thermal Stability of Thermoelectric Zn4Sb3. *Journal of Electronic Materials*, **2010**, 39, 1957-1959	1.9	36
363	In situ monitoring of TiO2(B)/anatase nanoparticle formation and application in Li-ion and Na-ion batteries. *Journal of Materials Chemistry A*, **2015**, 3, 18667-18674	13	35
362	Pulsed supercritical synthesis of anatase TiO□nanoparticles in a water-isopropanol mixture studied by in situ powder X-ray diffraction. *Nanoscale*, **2013**, 5, 2372-8	7.7	35
361	High-temperature thermoelectric properties of Cu1.97Ag0.03Se1+y. *Materials for Renewable and Sustainable Energy*, **2014**, 3, 1	4.7	34
360	Sintering and annealing effects on ZnO microstructure and thermoelectric properties. *Acta Materialia*, **2013**, 61, 3314-3323	8.4	34

359	Multipole electron-density modelling of synchrotron powder diffraction data: the case of diamond. *Acta Crystallographica Section A: Foundations and Advances*, **2010**, 66, 458-69		34
358	Mixed-terminal-ligand oxo-centered carboxylate-bridged trinuclear complexes: gas phase generation by means of electrospray ionization FT-ICR MS, condensed phase synthesis, and X-ray structure of K+[Cr3O(C6H5COO)6(F)2(H2O)]2(CH3)2CO. *Inorganica Chimica Acta*, **2001**, 319, 23-42	2.7	34
357	The Chemistry of Nucleation: In Situ Pair Distribution Function Analysis of Secondary Building Units During UiO-66 MOF Formation. *Chemistry - A European Journal*, **2019**, 25, 2051-2058	4.8	34
356	Direct Formation of Crystalline Phase Pure Rutile TiO2 Nanostructures by a Facile Hydrothermal Method. *Crystal Growth and Design*, **2013**, 13, 4730-4734	3.5	33
355	Watching nanoparticles form: an in situ (small-/wide-angle X-ray scattering/total scattering) study of the growth of yttria-stabilised zirconia in supercritical fluids. *Chemistry - A European Journal*, **2012**, 18, 5759-66	4.8	33
354	The effect of Mg doping on the thermoelectric performance of Zn4Sb3. *Journal of Applied Physics*, **2009**, 105, 013517	2.5	33
353	Errors in Maximum-Entropy Charge-Density Distributions Obtained from Diffraction Data. *Acta Crystallographica Section A: Foundations and Advances*, **1997**, 53, 376-387		33
352	Atomic displacement parameters for Ni(ND3)4(NO2)2 from 9 K X-ray and 13 K time-of-flight neutron diffraction data. *Acta Crystallographica Section B: Structural Science*, **1996**, 52, 923-931		33
351	Zn migration during spark plasma sintering of thermoelectric Zn4Sb3. *Applied Physics Letters*, **2012**, 101, 043901	3.4	32
350	Highly controlled crystallite size and crystallinity of pure and iron-doped anatase-TiO2 nanocrystals by continuous flow supercritical synthesis. *Journal of Materials Research*, **2013**, 28, 333-339	2.5	32
349	Real-time synchrotron powder X-ray diffraction study of the antisite defect formation during sub- and supercritical synthesis of LiFePO4and LiFe1MnxPO4nanoparticles. *Journal of Applied Crystallography*, **2011**, 44, 287-294	3.8	32
348	In-situ Synchrotron X-ray Diffraction Study of the Formation of Cubic Li2TiO3 Under Hydrothermal Conditions. *European Journal of Inorganic Chemistry*, **2011**, 2011, 2221-2226	2.3	32
347	Hydrothermal Liquefaction of Dried Distillers Grains with Solubles: A Reaction Temperature Study. *Energy & Fuels*, **2012**, 26, 5944-5953	4.1	31
346	Maximum-entropy-method charge densities based on structure-factor extraction with the commonly used Rietveld refinement programs GSAS, FullProf and Jana2006. *Acta Crystallographica Section A: Foundations and Advances*, **2012**, 68, 750-62		31
345	The rattler effect in thermoelectric clathrates studied by inelastic neutron scattering. *Physica B: Condensed Matter*, **2006**, 385-386, 505-507	2.8	31
344	Catalytic hydrotreatment of bio-crude produced from the hydrothermal liquefaction of aspen wood: a catalyst screening and parameter optimization study. *Sustainable Energy and Fuels*, **2017**, 1, 832-841	5.8	30
343	Hydrothermal Liquefaction of Enzymatic Hydrolysis Lignin: Biomass Pretreatment Severity Affects Lignin Valorization. *ACS Sustainable Chemistry and Engineering*, **2018**, 6, 5940-5949	8.3	30
342	Waterborne acrylic paint system based on nanoceria for corrosion protection of steel. *Progress in Organic Coatings*, **2016**, 96, 19-25	4.8	30

341	Electron-phonon coupling and surface Debye temperature of Bi2Te3(111) from helium atom scattering. *Physical Review B*, **2017**, 95,	3.3	30
340	Contemporary X-ray electron-density studies using synchrotron radiation. *IUCrJ*, **2014**, 1, 267-80	4.7	30
339	Photomagnetic switching of the complex [Nd(dmf)4(H2O)3(mu-CN)Fe(CN)5] x H2O analyzed by single-crystal X-ray diffraction. *Angewandte Chemie - International Edition*, **2009**, 48, 2780-3	16.4	30
338	Unchanged thermopower enhancement at the semiconductor-metal transition in correlated FeSb2−xTex. *Applied Physics Letters*, **2011**, 98, 072105	3.4	30
337	Synchrotron charge-density studies in materials chemistry: 16 K X-ray charge density of a new magnetic metal-organic framework material, [Mn2(C8H4O4)2(C3H7NO)2]. *Acta Crystallographica Section A: Foundations and Advances*, **2004**, 60, 382-9		30
336	Multitemperature Resonance-Diffraction and Structural Study of the Mixed-Valence Complex [Fe(3)O(OOCC(CH(3))(3))(6)(C(5)H(5)N)(3)]. *Inorganic Chemistry*, **1998**, 37, 6078-6083	5.1	30
335	High-Temperature Crystal Structure and Chemical Bonding in Thermoelectric Germanium Selenide (GeSe). *Chemistry - A European Journal*, **2017**, 23, 6888-6895	4.8	29
334	Fast direct synthesis and compaction of phase pure thermoelectric ZnSb. *Journal of Materials Chemistry C*, **2015**, 3, 10543-10553	7.1	29
333	Controlling Allotropism in Ruthenium Nanoparticles: A Pulsed-Flow Supercritical Synthesis and in Situ Synchrotron X-ray Diffraction Study. *Journal of Physical Chemistry C*, **2014**, 118, 11104-11110	3.8	29
332	Fast direct synthesis and compaction of homogenous phase-pure thermoelectric Zn4Sb3. *ACS Applied Materials & Interfaces*, **2014**, 6, 10542-8	9.5	29
331	Formation Mechanisms of Pt and Pt3Gd Nanoparticles under Solvothermal Conditions: An in Situ Total X-ray Scattering Study. *Journal of Physical Chemistry C*, **2015**, 119, 13357-13362	3.8	29
330	Characterization of Actinide Bonding in Th(S(2)PMe(2))(4) by Synchrotron X-ray Diffraction. *Inorganic Chemistry*, **1998**, 37, 4559-4566	5.1	29
329	Towards atomistic understanding of polymorphism in the solvothermal synthesis of ZrO nanoparticles. *Acta Crystallographica Section A: Foundations and Advances*, **2016**, 72, 645-650	1.7	28
328	High-power lithium-ion microbatteries from imprinted 3D electrodes of sub-10 nm LiMn2O4/Li4Ti5O12 nanocrystals and a copolymer gel electrolyte. *Nano Energy*, **2018**, 52, 431-440	17.1	28
327	X-Ray−neutron diffraction study of the electron-densitydistribution in trans-tetraaminedinitronickel(II) at9 K: transition-metal bonding and topological analysis. *Journal of the Chemical Society Dalton Transactions*, **1997**, 2227-2240		28
326	Synchrotron X-ray charge-density study of coordination polymer [Mn(HCOO)2(H2O)2]infinity. *Chemistry - A European Journal*, **2007**, 13, 9775-90	4.8	28
325	Covalent Guest−Framework Interactions in Heavy Metal Sodalites: Structure and Properties of Thallium and Silver Sodalite. *Journal of Physical Chemistry B*, **1999**, 103, 7135-7144	3.4	28
324	Atomic and electronic structure transformations in SnS2 at high pressures: a joint single crystal X-ray diffraction and DFT study. *Dalton Transactions*, **2016**, 45, 3798-805	4.3	27

323	Pushing X-ray electron densities to the limit: thermoelectric CoSb3. *Angewandte Chemie - International Edition*, **2013**, 52, 1503-6	16.4	27
322	Comparative study of X-ray charge-density data on CoSb3. *Acta Crystallographica Section A: Foundations and Advances*, **2013**, 69, 570-82		27
321	Multi-temperature synchrotron PXRD and physical properties study of half-Heusler TiCoSb. *Dalton Transactions*, **2010**, 39, 10154-9	4.3	27
320	X-ray charge density study of chemical bonding in skutterudite CoSb3. *Physical Review B*, **2007**, 76,	3.3	27
319	Structural study of Fe doped and Ni substituted thermoelectric skutterudites by combined synchrotron and neutron powder diffraction and ab initio theory. *Journal of Applied Physics*, **2004**, 96, 3148-3157	2.5	27
318	X-ray and neutron diffraction study of benzoylacetone in the temperature range 8-300 K: comparison with other cis-enol molecules. *Acta Crystallographica Section B: Structural Science*, **1999**, 55, 767-787		27
317	Order-disorder transition in nano-rutile TiO anodes: a high capacity low-volume change Li-ion battery material. *Nanoscale*, **2019**, 11, 12347-12357	7.7	26
316	Development of a Dual-Stage Continuous Flow Reactor for Hydrothermal Synthesis of Hybrid Nanoparticles. *Industrial & Engineering Chemistry Research*, **2015**, 54, 8500-8508	3.9	26
315	Effect of gas pressure on negative thermal expansion in MOF-5. *Chemical Communications*, **2013**, 49, 789-91	5.8	26
314	Bonded radii and the contraction of the electron density of the oxygen atom by bonded interactions. *Journal of Physical Chemistry A*, **2013**, 117, 1632-40	2.8	26
313	Comparison of T-piece and concentric mixing systems for continuous flow synthesis of anatase nanoparticles in supercritical isopropanol/water. *Journal of Solid State Chemistry*, **2009**, 182, 491-495	3.3	26
312	Fast Preparation and Characterization of Quarternary Thermoelectric Clathrates. *Chemistry of Materials*, **2009**, 21, 122-127	9.6	26
311	A direct investigation of thermal vibrations of beryllium in real space through the maximum-entropy method applied to single-crystal neutron diffraction data. *Acta Crystallographica Section A: Foundations and Advances*, **1994**, 50, 330-337		26
310	The chemistry of ZnWO nanoparticle formation. *Chemical Science*, **2016**, 7, 6394-6406	9.4	26
309	Structural disorder, anisotropic micro-strain and cation vacancies in thermo-electric lead chalcogenides. *Physical Chemistry Chemical Physics*, **2016**, 18, 15874-83	3.6	25
308	Using design of experiments to optimize derivatization with methyl chloroformate for quantitative analysis of the aqueous phase from hydrothermal liquefaction of biomass. *Analytical and Bioanalytical Chemistry*, **2016**, 408, 2171-83	4.4	25
307	Alkali metal ion templated transition metal formate framework materials: synthesis, crystal structures, ion migration, and magnetism. *Inorganic Chemistry*, **2014**, 53, 10178-88	5.1	25
306	Phase transition of [2,2]-paracyclophane--an end to an apparently endless story. *Chemistry - A European Journal*, **2014**, 20, 7048-53	4.8	25

305	Rapid one-step low-temperature synthesis of nanocrystalline Al2O3. *Angewandte Chemie - International Edition*, **2011**, 50, 7045-7	16.4	25
304	Clathrate guest atoms under pressure. *Journal of Applied Physics*, **2009**, 105, 073508	2.5	25
303	Effects of weak intermolecular interactions on the molecular isomerism of tricobalt metal chains. *Journal of the American Chemical Society*, **2009**, 131, 7580-91	16.4	25
302	Electronic structure of the sodium and potassium electrosodalites (Na/K)8(AlSiO4)6. *Physical Review B*, **2001**, 64,	3.3	25
301	Enhanced thermoelectric performance and high-temperature thermal stability of p-type Ag-doped Zn4Sb3. *Journal of Materials Chemistry A*, **2018**, 6, 4079-4087	13	24
300	Nanoscale surface dynamics of BiTe(111): observation of a prominent surface acoustic wave and the role of van der Waals interactions. *Nanoscale*, **2018**, 10, 14627-14636	7.7	24
299	Intra- and interband electron scattering in a hybrid topological insulator: Bismuth bilayer on Bi2Se3. *Physical Review B*, **2014**, 90,	3.3	24
298	Investigation of the precipitation of Na2SO4 in supercritical water. *Chemical Engineering Science*, **2017**, 174, 268-276	4.4	24
297	Formation and Growth of Bi2Te3 in Biomolecule-Assisted Near-Critical Water: In Situ Synchrotron Radiation Study. *Journal of Physical Chemistry C*, **2010**, 114, 12133-12138	3.8	24
296	NMR Knight shifts and the electronic properties of Rb8Na16Si136 clathrate. *Physical Review B*, **2001**, 63,	3.3	24
295	Guide to by-products formed in organic solvents under solvothermal conditions. *Journal of Supercritical Fluids*, **2016**, 113, 166-197	4.2	24
294	Thermal stability of Mg3Sb1.475Bi0.475Te0.05 high performance n-type thermoelectric investigated through powder X-ray diffraction and pair distribution function analysis. *Journal of Materials Chemistry A*, **2018**, 6, 17171-17176	13	23
293	Evolution of magnetic and structural transitions and enhancement of magnetocaloric effect in Fe1MnxV2O4. *Physical Review B*, **2014**, 89,	3.3	23
292	Simple method for manufacturing Pt counter electrodes on conductive plastic substrates for dye-sensitized solar cells. *ACS Applied Materials & Interfaces*, **2013**, 5, 795-800	9.5	23
291	Thermal stability and thermoelectric properties of Mg2Si0.4Sn0.6 and Mg2Si0.6Sn0.4. *Journal of Materials Science*, **2013**, 48, 2002-2008	4.3	23
290	Multi-temperature Synchrotron Powder X-ray Diffraction Study and Hirshfeld Surface Analysis of Chemical Bonding in the Thermoelectric Zintl Phase Yb14MnSb11. *Chemistry of Materials*, **2011**, 23, 3723-3730	9.6	23
289	Thermoelectric transport properties of highly oriented FeSb2 thin films. *Journal of Applied Physics*, **2009**, 106, 033710	2.5	23
288	Measurement of Electric Fields Experienced by Urea Guest Molecules in the 18-Crown-6/Urea (1:5) Host-Guest Complex: An Experimental Reference Point for Electric-Field-Assisted Catalysis. *Journal of the American Chemical Society*, **2019**, 141, 3965-3976	16.4	23

287	TiO2 Nanoparticles for Li-Ion Battery Anodes: Mitigation of Growth and Irreversible Capacity Using LiOH and NaOH. *Chemistry of Materials*, **2015**, 27, 119-126	9.6	22
286	Highly dispersive electron relaxation and colossal thermoelectricity in the correlated semiconductor FeSb2. *Physical Review B*, **2013**, 88,	3.3	22
285	Thermal Stability of High Performance Thermoelectric Zn4Sb3 in Argon. *European Journal of Inorganic Chemistry*, **2011**, 2011, 2733-2737	2.3	22
284	Strong electron correlations in FeSb2: An optical investigation and comparison with RuSb2. *Physical Review B*, **2010**, 82,	3.3	22
283	Thermoelectric Characteristics of Electrochemically Deposited Bi2Te3and Sb2Te3Thin Films of Relevance to Multilayer Preparation. *Journal of the Electrochemical Society*, **2011**, 159, D50-D58	3.9	22
282	Photomagnetic switching of heterometallic complexes [M(dmf)4(H2O)3(mu-CN)Fe(CN)5].H2O (M=Nd, La, Gd, Y) analyzed by single-crystal X-ray diffraction and ab initio theory. *Chemistry - A European Journal*, **2010**, 16, 7215-23	4.8	22
281	Effect of Aqueous Phase Recycling in Continuous Hydrothermal Liquefaction. *Industrial & Engineering Chemistry Research*, **2016**, 55, 12317-12325	3.9	21
280	Glass-like thermal conductivity gradually induced in thermoelectric Sr8Ga16Ge30 clathrate by off-centered guest atoms. *Journal of Applied Physics*, **2016**, 119, 185102	2.5	21
279	Hydrothermal Synthesis of CoSb2O4: In Situ Powder X-ray Diffraction, Crystal Structure, and Electrochemical Properties. *Crystal Growth and Design*, **2016**, 16, 834-841	3.5	21
278	Gravity-induced gradients in thermoelectric Mg2Si0.9925SnxSb0.0075. *Acta Materialia*, **2012**, 60, 5745-5751	5.4	21
277	Copper doped TiO2 nanoparticles characterized by X-ray absorption spectroscopy, total scattering, and powder diffraction--a benchmark structure-property study. *Dalton Transactions*, **2013**, 42, 9555-64	4.3	21
276	Structure, Size, and Morphology Control of Nanocrystalline Lithium Cobalt Oxide. *Crystal Growth and Design*, **2011**, 11, 753-758	3.5	21
275	In situ high-energy synchrotron radiation study of boehmite formation, growth, and phase transformation to alumina in sub- and supercritical water. *Chemistry - A European Journal*, **2009**, 15, 13381-90	4.8	21
274	Enhanced thermoelectric performance in rare-earth filled-skutterudites. *Journal of Materials Chemistry C*, **2016**, 4, 4374-4379	7.1	21
273	Reorientation of the diagonal double-stripe spin structure at FeTe bulk and thin-film surfaces. *Nature Communications*, **2017**, 8, 13939	17.4	20
272	The formation mechanism of bimetallic PtRu alloy nanoparticles in solvothermal synthesis. *Nanoscale*, **2015**, 7, 16170-4	7.7	20
271	Pitfalls and reproducibility ofin situsynchrotron powder X-ray diffraction studies of solvothermal nanoparticle formation. *Journal of Applied Crystallography*, **2018**, 51, 526-540	3.8	20
270	Hydrothermal liquefaction of Miscanthus Giganteus: Preparation of the ideal feedstock. *Biomass and Bioenergy*, **2016**, 87, 17-25	5.3	20

269	Fermi surface complexity, effective mass, and conduction band alignment in n-type thermoelectric Mg3Sb2 xBix from first principles calculations. *Journal of Applied Physics*, **2019**, 126, 085104	2.5	20
268	Characterization of the interface between an Fe Cr alloy and the p-type thermoelectric oxide Ca3Co4O9. *Journal of Alloys and Compounds*, **2014**, 582, 827-833	5.7	20
267	Thermoelectric studies in Zn4Sb3 the complex interdependence between thermal stability, thermoelectric transport, and zinc content. *Journal of Applied Physics*, **2013**, 113, 103708	2.5	20
266	Highly enhanced thermal stability of Zn4Sb3 nanocomposites. *Chemical Communications*, **2013**, 49, 6540-28	5.8	20
265	An electrochemical cell for in operando studies of lithium/sodium batteries using a conventional x-ray powder diffractometer. *Review of Scientific Instruments*, **2014**, 85, 104103	1.7	20
264	Experimental Electron Density Studies of Inorganic Materials. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2013**, 639, 1922-1932	1.3	20
263	Intermolecular interactions and electrostatic properties of the hydroquinone apohost: implications for supramolecular chemistry. *Journal of Physical Chemistry A*, **2011**, 115, 12962-72	2.8	20
262	The Debye-Scherrer camera at synchrotron sources: a revisit. *Journal of Synchrotron Radiation*, **2013** , 20, 98-104	2.4	19
261	Redox-Driven Migration of Copper Ions in the Cu-CHA Zeolite as Shown by the In Situ PXRD/XANES Technique. *Angewandte Chemie*, **2017**, 129, 10503-10508	3.6	19
260	Mesoporous TiO2 aggregate photoanode with high specific surface area and strong light scattering for dye-sensitized solar cells. *Journal of Solid State Chemistry*, **2012**, 196, 504-510	3.3	19
259	Barium dynamics in noble-metal clathrates. *Physical Review B*, **2010**, 82,	3.3	19
258	Thermoelectric properties of the narrow-gap semiconductors FeSb2and RuSb2: A comparative study. *Journal of Physics: Conference Series*, **2009**, 150, 012049	0.3	19
257	Continuous flow supercritical water synthesis and crystallographic characterization of anisotropic boehmite nanoparticles. *Journal of Applied Crystallography*, **2010**, 43, 858-866	3.8	19
256	Importance of True Satellite Reflections in the Analysis of Modulated, Composite Crystal Structures. I. A New Refinement of [M 2Cu2O3]7+[CuO2]10, M = Bi0.06Sr0.46Ca0.48. *Acta Crystallographica Section B: Structural Science*, **1997**, 53, 113-124		19
255	Solvothermal synthesis, multi-temperature crystal structures and physical properties of isostructural coordination polymers, 2C4H12N+[M3(C8H4O4)4]2-.3C5H11NO, M = Co, Zn. *Acta Crystallographica Section B: Structural Science*, **2006**, 62, 245-54		19
254	Solving the disordered structure of CuSe using the three-dimensional difference pair distribution function. *Acta Crystallographica Section A: Foundations and Advances*, **2019**, 75, 465-473	1.7	18
253	Enhanced thermoelectric properties of SnSe thin films grown by single-target magnetron sputtering. *Journal of Materials Chemistry A*, **2019**, 7, 17981-17986	13	18
252	Analysis of the photomagnetic properties of cyano-bridged heterobimetallic complexes by X-ray diffraction. *Inorganic Chemistry*, **2011**, 50, 10974-84	5.1	18

251	Experimental and theoretical charge-density study of a tetranuclear cobalt carbonyl complex. *Acta Crystallographica Section B: Structural Science*, **2009**, 65, 715-23		18
250	Growth of FeSb2 thin films by magnetron sputtering. *Thin Solid Films*, **2011**, 519, 5397-5402	2.2	18
249	Highly Selective Deethylation of Rhodamine B on Prepared in Supercritical Fluids. *International Journal of Photoenergy*, **2012**, 2012, 1-7	2.1	18
248	Helium cryostat synchrotron charge densities determined using a large CCD detector the upgraded beamline D3 at DESY. *Journal of Applied Crystallography*, **2008**, 41, 846-853	3.8	18
247	Reciprocal- and direct-space determination of the temperature dependence of thermal vibrations in magnesium: A neutron diffraction study. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, **1995**, 72, 1357-1380		18
246	Formation mechanism and growth of MNbO3, M=K, Na by in situ X-ray diffraction. *Journal of the American Ceramic Society*, **2017**, 100, 3835-3842	3.8	17
245	Intermolecular Interaction Energies in Hydroquinone Clathrates at High Pressure. *Crystal Growth and Design*, **2017**, 17, 3834-3846	3.5	17
244	Synchrotron powder diffraction of silicon: high-quality structure factors and electron density. *Acta Crystallographica Section A: Foundations and Advances*, **2016**, 72, 28-35	1.7	17
243	Functionally Graded Ge1 Six Thermoelectrics by Simultaneous Band Gap and Carrier Density Engineering. *Chemistry of Materials*, **2014**, 26, 4992-4997	9.6	17
242	Experimental and theoretical charge densities of a zinc-containing coordination polymer, Zn(HCOO)2(H2O)2. *Inorganic Chemistry*, **2013**, 52, 297-305	5.1	17
241	Thermoelectric Properties of the Entire Composition Range in Mg2Si0.9925 Sn x Sb0.0075. *Journal of Electronic Materials*, **2013**, 42, 1417-1421	1.9	17
240	Chemical bonding in a linear chromium metal string complex. *Inorganic Chemistry*, **2014**, 53, 12489-98	5.1	17
239	Multitemperature synchrotron powder diffraction and thermoelectric properties of the skutterudite La0.1Co4Sb12. *Journal of Applied Physics*, **2010**, 107, 113507	2.5	17
238	A crystalline microporous narrow-bandgap semiconductor. *Angewandte Chemie - International Edition*, **2004**, 43, 700-4	16.4	17
237	Rapid One-Step Synthesis and Compaction of High-Performance n-Type Mg Sb Thermoelectrics. *Angewandte Chemie - International Edition*, **2020**, 59, 4278-4282	16.4	17
236	Carrier concentration dependence of structural disorder in thermoelectric Sn Te. *IUCrJ*, **2016**, 3, 377-388	4.7	17
235	Insights into BaTi1 ZryO3 (0 y 1) Synthesis under Supercritical Fluid Conditions. *Chemistry of Materials*, **2016**, 28, 3391-3400	9.6	17
234	Resonant Plasmon-Enhanced Upconversion in Monolayers of Core-Shell Nanocrystals: Role of Shell Thickness. *ACS Applied Materials & Interfaces*, **2019**, 11, 1209-1218	9.5	17

233	Strategies for synthesis of Prussian blue analogues. *Royal Society Open Science*, **2021**, 8, 201779	3.3	17
232	Thermal stability of p-type Ag-doped MgSb thermoelectric materials investigated by powder X-ray diffraction. *Physical Chemistry Chemical Physics*, **2019**, 21, 4295-4305	3.6	16
231	Hydrothermal Synthesis and in Situ Powder X-ray Diffraction Study of Bismuth-Substituted Ceria Nanoparticles. *Crystal Growth and Design*, **2015**, 15, 3628-3636	3.5	16
230	Structural Evolution of Iron Antimonides from Amorphous Precursors to Crystalline Products Studied by Total Scattering Techniques. *Journal of the American Chemical Society*, **2015**, 137, 9652-8	16.4	16
229	Powder X-ray Diffraction Electron Density of Cubic Boron Nitride. *Journal of Physical Chemistry C*, **2015**, 119, 6164-6173	3.8	16
228	Electron Density Studies in Materials Research. *Chemistry - A European Journal*, **2019**, 25, 15010-15029	4.8	16
227	Molecular Imprisonment: Host Response to Guest Location, Orientation, and Dynamics in Clathrates of Dianin□s Compound. *Crystal Growth and Design*, **2014**, 14, 1296-1306	3.5	16
226	(NH4)4Sn2S6□3H2O: Crystal Structure, Thermal Decomposition, and Precursor for Textured Thin Film. *Chemistry of Materials*, **2014**, 26, 4494-4504	9.6	16
225	Characterization of a multicomponent lithium lithiate from a combined x-ray diffraction, NMR spectroscopy, and computational approach. *Angewandte Chemie - International Edition*, **2014**, 53, 13282-7	16.4	16
224	Host□guest coupling in semiconducting Ba8Zn8Ge38. *Journal of Physics Condensed Matter*, **2008**, 20, 104244	1.8	16
223	In Situ High-Energy Synchrotron Radiation Study of Sol□el Nanoparticle Formation in Supercritical Fluids. *Angewandte Chemie*, **2007**, 119, 1131-1134	3.6	16
222	Autocatalytic Formation of High-Entropy Alloy Nanoparticles. *Angewandte Chemie - International Edition*, **2020**, 59, 21920-21924	16.4	16
221	Products of hydrothermal treatment of lignin and the importance of ortho-directed repolymerization reactions. *Journal of Analytical and Applied Pyrolysis*, **2017**, 126, 371-379	6	15
220	Rationalization of Hydrothermal Synthesis of NaNbO3 by Rapid in Situ Time-Resolved Synchrotron X-ray Diffraction. *Crystal Growth and Design*, **2018**, 18, 770-774	3.5	15
219	Relating phase transition heat capacity to thermal conductivity and effusivity in Cu2Se. *Physica Status Solidi - Rapid Research Letters*, **2016**, 10, 618-621	2.5	15
218	Synchrotron Powder Diffraction at P02.1 at PETRA III: From Electron Density Distributions to in situ Total Scattering. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2014**, 640, 3094-3099	1.3	15
217	Glucose-assisted continuous flow synthesis of Bi2Te3 nanoparticles in supercritical/near-critical water. *Journal of Supercritical Fluids*, **2012**, 67, 84-88	4.2	15
216	Elaborating the Crystal Structures of MgAgSb Thermoelectric Compound: Polymorphs and Atomic Disorders. *Chemistry of Materials*, **2017**, 29, 6378-6388	9.6	15

215	Crystal structure and chemical bonding of the intermetallic Zintl phase Yb11AlSb9. *Dalton Transactions*, **2012**, 41, 10347-53	4.3	15
214	Application of atomic Hirshfeld surface analysis to intermetallic systems: is Mn in cubic CeMnNi4 a thermoelectric rattler atom?. *Inorganic Chemistry*, **2012**, 51, 1916-24	5.1	15
213	On the significance of Bragg reflections. *Acta Crystallographica Section A: Foundations and Advances* , **2012**, 68, 301-3; discussion 304		15
212	Structural Collapse of the Hydroquinone-Formic Acid Clathrate: A Pressure-Medium-Dependent Phase Transition. *Chemistry - A European Journal*, **2016**, 22, 4061-9	4.8	15
211	In Situ PDF Study of the Nucleation and Growth of Intermetallic PtPb Nanocrystals. *ChemNanoMat*, **2017**, 3, 472-478	3.5	14
210	Nuclear-weighted X-ray maximum entropy method - NXMEM. *Acta Crystallographica Section A: Foundations and Advances*, **2015**, 71, 9-19	1.7	14
209	Core-shell nanoparticles by silica coating of metal oxides in a dual-stage hydrothermal flow reactor. *Chemical Communications*, **2016**, 52, 3434-7	5.8	14
208	In situ synchrotron powder X-ray diffraction study of formation and growth of yttrium and ytterbium aluminum garnet nanoparticles in sub- and supercritical water. *RSC Advances*, **2013**, 3, 15368	3.7	14
207	Measuring anisotropic resistivity of single crystals using the van der Pauw technique. *Physical Review B*, **2015**, 92,	3.3	14
206	Optimised photocatalytic hydrogen production using core-shell AuPd promoters with controlled shell thickness. *Physical Chemistry Chemical Physics*, **2014**, 16, 26638-44	3.6	14
205	High-temperature and high-pressure pulsed synthesis apparatus for supercritical production of nanoparticles. *Review of Scientific Instruments*, **2011**, 82, 084102	1.7	14
204	Thermoelectric Characterization of Zone-Melted and Quenched Zn4Sb3. *Journal of Electronic Materials*, **2010**, 39, 1975-1980	1.9	14
203	Time-resolved grazing-incidence pair distribution functions during deposition by radio-frequency magnetron sputtering. *IUCrJ*, **2019**, 6, 299-304	4.7	14
202	A simple model for vacancy order and disorder in defective half-Heusler systems. *IUCrJ*, **2020**, 7, 673-680	4.7	14
201	Unraveling the spin structure of unoccupied states in Bi2Se3. *Physical Review B*, **2017**, 95,	3.3	13
200	Expanding the structural versatility of thiostannate(IV) complexes. *CrystEngComm*, **2015**, 17, 2413-2420	3.3	13
199	Crystal structure, microstructure and electrochemical properties of hydrothermally synthesised LiMn2O4. *CrystEngComm*, **2016**, 18, 1996-2004	3.3	13
198	Orientation control and thermoelectric properties of FeSb2films. *Journal Physics D: Applied Physics*, **2010**, 43, 205402	3	13

197	The cation-vacancy ordering transition in dehydrated Na6 sodalite. *Journal of Chemical Physics*, **2000**, 113, 10226-10239	3.9	13
196	Structural stability and thermoelectric properties of cation- and anion-doped Mg2Si0.4Sn0.6. *Inorganic Chemistry Frontiers*, **2017**, 4, 456-467	6.8	12
195	Reconciling Crystallographic and Physical Property Measurements on Thermoelectric Lead Sulfide. *Journal of the American Chemical Society*, **2019**, 141, 8146-8157	16.4	12
194	Crystal Structure of Thecotrichite, an Efflorescent Salt on Calcareous Objects Stored in Wooden Cabinets. *Crystal Growth and Design*, **2015**, 15, 2795-2800	3.5	12
193	Detailed Investigation into the Asphaltene Fraction of Hydrothermal Liquefaction Derived Bio-Crude and Hydrotreated Bio-Crudes. *Energy & Fuels*, **2018**, 32, 3579-3587	4.1	12
192	Screening and atomic-scale engineering of the potential at a topological insulator surface. *Physical Review B*, **2014**, 89,	3.3	12
191	Pressure versus temperature effects on intramolecular electron transfer in mixed-valence complexes. *Chemistry - A European Journal*, **2013**, 19, 195-205	4.8	12
190	In Operando Study of High-Performance Thermoelectric Materials for Power Generation: A Case Study of Zn4sb3. *Advanced Electronic Materials*, **2017**, 3, 1700223	6.4	12
189	Strongly anisotropic spin-orbit splitting in a two-dimensional electron gas. *Physical Review B*, **2015**, 91,	3.3	12
188	Strong electron correlations in FeSb2. *Annalen Der Physik*, **2011**, 523, 612-620	2.6	12
187	Phonon properties in narrow gap FeSi and FeSb2 single crystals. *Journal of Applied Physics*, **2008**, 103, 07C912	2.5	12
186	Single-Crystal Neutron Diffraction Study of Diammonium Hexaaquacopper Disulfate at 15 and 293 K. Investigation of Anharmonic Thermal Motion.. *Acta Chemica Scandinavica*, **1994**, 48, 800-809		12
185	Dipole-Oriented Molecular Solids Can Undergo a Phase Change and Still Maintain Electrical Polarization. *Journal of Physical Chemistry C*, **2016**, 120, 24130-24136	3.8	12
184	Functionally Graded (PbTe)1(SnTe)x Thermoelectrics. *Chemistry of Materials*, **2018**, 30, 280-287	9.6	12
183	Low-Temperature Anharmonicity in Cesium Chloride (CsCl). *Angewandte Chemie - International Edition*, **2017**, 56, 3625-3629	16.4	11
182	Revealing the slow decomposition kinetics of type-I clathrate BaGaGe. *Physical Chemistry Chemical Physics*, **2017**, 19, 15734-15744	3.6	11
181	In operando observation of sodium ion diffusion in a layered sodium transition metal oxide cathode material, P2 NaCoMnO. *Chemical Communications*, **2017**, 53, 1160-1163	5.8	11
180	Analysis of organic gas phase compounds formed by hydrothermal liquefaction of Dried Distillers Grains with Solubles. *Bioresource Technology*, **2015**, 192, 826-30	11	11

179	Accurate high-resolution single-crystal diffraction data from a Pilatus3 X CdTe detector. *Journal of Applied Crystallography*, **2020**, 53, 635-649	3.8	11
178	Sputtering-induced reemergence of the topological surface state in Bi2Se3. *Physical Review B*, **2016**, 93,	3.3	11
177	Quantifying Host□Guest Interaction Energies in Clathrates of Dianin□s Compound. *Crystal Growth and Design*, **2016**, 16, 6858-6866	3.5	11
176	Pauling bond strength, bond length and electron density distribution. *Physics and Chemistry of Minerals*, **2014**, 41, 17-25	1.6	11
175	Expression and interactions of stereochemically active lone pairs and their relation to structural distortions and thermal conductivity. *IUCrJ*, **2020**, 7, 480-489	4.7	11
174	Bismuth Iodide Hybrid Organic-Inorganic Crystal Structures and Utilization in Formation of Textured BiI3 Film. *European Journal of Inorganic Chemistry*, **2016**, 2016, 1389-1394	2.3	11
173	High-temperature thermoelectric properties of Ca0.9Y0.1Mn1□ Fe x O3 (0 □x □0.25). *Journal of Materials Science*, **2013**, 48, 2817-2822	4.3	10
172	Accurate atomic displacement parameters from time-of-flight neutron-diffraction data at TOPAZ. *Acta Crystallographica Section A: Foundations and Advances*, **2014**, 70, 679-681	1.7	10
171	Understanding the Formation and Evolution of Ceria Nanoparticles Under Hydrothermal Conditions. *Angewandte Chemie*, **2012**, 124, 9164-9167	3.6	10
170	Rapid Synthesis of Porous, Mixed Phase Titania Films with Tailored Orientation of Rutile for Enhanced Photocatalytic Performance. *Journal of Physical Chemistry C*, **2013**, 117, 27039-27046	3.8	10
169	Model-free reconstruction of magnetic correlations in frustrated magnets. *IUCrJ*, **2018**, 5, 410-416	4.7	10
168	Charge Density Methods in Hydrogen Bond Studies. *Structure and Bonding*, **2010**, 53-74	0.9	10
167	Continuous flow hydrothermal synthesis of rutile SnO2 nanoparticles: Exploration of pH and temperature effects. *Journal of Supercritical Fluids*, **2020**, 166, 105029	4.2	10
166	Improved Thermoelectric Properties of N-Type MgSb through Cation-Site Doping with Gd or Ho. *ACS Applied Materials & Interfaces*, **2021**, 13, 10964-10971	9.5	10
165	Structural Evolution of Aqueous Zirconium Acetate by Time-Resolved Small-Angle X-ray Scattering and Rheology. *Journal of Physical Chemistry C*, **2015**, 119, 12660-12667	3.8	9
164	High pressure induced charge transfer in 3d-4f bimetallic photomagnetic materials. *Chemical Communications*, **2015**, 51, 8868-71	5.8	9
163	Fine tunable aqueous solution synthesis of textured flexible SnS2 thin films and nanosheets. *Physical Chemistry Chemical Physics*, **2015**, 17, 9282-7	3.6	9
162	High-pressure single crystal X-ray diffraction study of the linear metal chain compound Co3(dpa)4Br2□CH2Cl2. *Dalton Transactions*, **2015**, 44, 9038-43	4.3	9

161	Atomic Scale Design of Spinel ZnAl2O4 Nanocrystal Synthesis. *Crystal Growth and Design*, **2020**, 20, 1789-1799	3.9	9
160	Promotion Mechanisms of Au Supported on TiO2 in Thermal- and Photocatalytic Glycerol Conversion. *Journal of Physical Chemistry C*, **2019**, 123, 19734-19741	3.8	9
159	A structural study of a three-membered linear metal chain compound at elevated pressure. *Dalton Transactions*, **2014**, 43, 1313-20	4.3	9
158	A Theoretical Study on the Rotational Motion and Interactions in the Disordered Phase of MBH4 (M = Li, Na, K, Rb, Cs). *Journal of Physical Chemistry C*, **2013**, 117, 2308-2316	3.8	9
157	Temperature-dependent crystal structure of the isopropanol clathrate of Dianin's compound. *Chemical Communications*, **2011**, 47, 2029-31	5.8	9
156	Experimental charge density in an oxidized trinuclear iron complex using 15 K synchrotron and 100 K conventional single-crystal X-ray diffraction. *Dalton Transactions*, **2009**, 664-71	4.3	9
155	Surfactant-free synthesis of nickel nanoparticles in near-critical water. *Journal of Solid State Chemistry*, **2008**, 181, 2681-2683	3.3	9
154	Crystal and magnetic structure of Eu4Ga8Ge16. *Physical Review B*, **2003**, 68,	3.3	9
153	Microstructure and Thermoelectric Properties of Zn1−xAgxSb Thin Films Grown by Single-Target Magnetron Sputtering. *ACS Applied Energy Materials*, **2020**, 3, 2055-2062	6.1	9
152	Probing Efficient N-Type Lanthanide Dopants for MgSb Thermoelectrics. *Advanced Science*, **2020**, 7, 2002867	15.7	9
151	Thermoelectric materials with crystal-amorphicity duality induced by large atomic size mismatch. *Joule*, **2021**, 5, 1183-1195	27.8	9
150	Alkali Counterions Impact Crystallization Kinetics of Apatite Nanocrystals from Amorphous Calcium Phosphate in Water at High pH. *Crystal Growth and Design*, **2018**, 18, 6723-6728	3.5	9
149	Boosting Photocatalytic Hydrogen Production by Modulating Recombination Modes and Proton Adsorption Energy. *Journal of Physical Chemistry Letters*, **2019**, 10, 5381-5386	6.4	8
148	Low-Barrier Hydrogen Bonds in Negative Thermal Expansion Material H [Co(CN)]. *Chemistry - A European Journal*, **2019**, 25, 6814-6822	4.8	8
147	Well-controlled metal co-catalysts synthesised by chemical vapour impregnation for photocatalytic hydrogen production and water purification. *Dalton Transactions*, **2014**, 43, 14976-82	4.3	8
146	In situ powder X-ray diffraction study of the hydro-thermal formation of LiMn2O4 nanocrystallites. *Dalton Transactions*, **2014**, 43, 15075-84	4.3	8
145	Host perturbation in a β-hydroquinone clathrate studied by combined X-ray/neutron charge-density analysis: implications for molecular inclusion in supramolecular entities. *Chemistry - A European Journal*, **2014**, 20, 8089-98	4.8	8
144	Multi-temperature structure of thermoelectric Mg2Si and Mg2Sn. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2017**, 73, 1158-1163	1.8	8

143	Pulsed-Flow Near-Critical and Supercritical Synthesis of Carbon-Supported Platinum Nanoparticles and In Situ X-ray Diffraction Study of Their Formation and Growth. *Chemistry of Materials*, **2015**, 27, 450-456	9.6	8
142	Investigation of the correlation between stoichiometry and thermoelectric properties in a PtSb2 single crystal. *Dalton Transactions*, **2012**, 41, 1278-83	4.3	8
141	Growth and thermoelectric properties of FeSb2 films produced by pulsed laser deposition. *Applied Physics A: Materials Science and Processing*, **2011**, 104, 883-887	2.6	8
140	Thermoelectric and microstructural properties of Pb0.9Sn0.1GexTe compounds prepared by spinodal decomposition. *Journal of Solid State Chemistry*, **2011**, 184, 1172-1175	3.3	8
139	Multiple phase formation and its influence on lattice thermal conductivity in Zn4Sb3. *Journal of Materials Research*, **2011**, 26, 1925-1932	2.5	8
138	Colossal Seebeck coefficient in strongly correlated semiconductor FeSb 2. *Europhysics Letters*, **2007** , 80, 39901	1.6	8
137	Testing theory beyond molecular structure: Electron density distributions of complex molecules. *International Journal of Quantum Chemistry*, **2004**, 96, 23-31	2.1	8
136	Magnetic phase diagram of Eu4Ga8Ge16 by magnetic susceptibility, heat capacity, and Mssbauer measurements. *Physical Review B*, **2003**, 68,	3.3	8
135	Anisotropic compressibility of the coordination polymer emim[Mn(btc)]. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2016**, 72, 389-94	1.8	8
134	Electron Density Analysis of the "O-O" Charge-Shift Bonding in Rubrene Endoperoxide. *Journal of Physical Chemistry A*, **2016**, 120, 7510-8	2.8	8
133	Breaking thermoelectric performance limits. *Nature Materials*, **2021**, 20, 1309-1310	27	8
132	Accurate charge densities from powder X-ray diffraction - a new version of the Aarhus vacuum imaging-plate diffractometer. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2017**, 73, 521-530	1.8	7
131	Formation Mechanism of Epitaxial PalladiumPlatinum CoreShell Nanocatalysts in a One-Step Supercritical Synthesis. *Advanced Functional Materials*, **2019**, 29, 1902214	15.6	7
130	Mapping the complete bonding network in KBH4 using the combined power of powder diffraction and maximum entropy method. *Computational and Theoretical Chemistry*, **2015**, 1053, 245-253	2	7
129	A Helium-Surface Interaction Potential of Bi2Te3(111) from Ultrahigh-Resolution Spin-Echo Measurements. *Surface Science*, **2018**, 678, 25-31	1.8	7
128	Nickel: The time-reversal symmetry conserving partner of iron on a chalcogenide topological insulator. *Physical Review B*, **2016**, 94,	3.3	7
127	Chemometric analysis of composition of bio-crude and aqueous phase from hydrothermal liquefaction of thermally and chemically pretreated Miscanthus x giganteus. *Biomass and Bioenergy*, **2016**, 95, 137-145	5.3	7
126	Low-temperature powder X-ray diffraction measurements in vacuum: analysis of the thermal displacement of copper. *Journal of Applied Crystallography*, **2016**, 49, 110-119	3.8	7

125	In Situ Total X-Ray Scattering Study of WO3 Nanoparticle Formation under Hydrothermal Conditions. *Angewandte Chemie*, **2014**, 126, 3741-3744	3.6	7
124	Tailoring band gap and thermal diffusivity of nanostructured phase-pure ZnAl2O4 by direct spark plasma sintering synthesis. *Journal of Solid State Chemistry*, **2017**, 256, 45-52	3.3	7
123	Assessment of agricultural crops and natural vegetation in Scotland for energy production by anaerobic digestion and hydrothermal liquefaction. *Biomass Conversion and Biorefinery*, **2017**, 7, 467-477	2.3	7
122	Insight into Nucleation and Growth of Bi2□SbxTe3 (x = 0□) Nanoplatelets in Hydrothermal Synthesis. *Chemistry of Materials*, **2017**, 29, 5070-5079	9.6	7
121	Effect of Thermal Cycling on Zinc Antimonide Thin Film Thermoelectric Characteristics. *Energy Procedia*, **2017**, 142, 519-524	2.3	7
120	Sb Magnetic Resonance as a Local Probe for the Gap Formation in the Correlated Semimetal FeSb2. *Applied Magnetic Resonance*, **2014**, 45, 1237-1252	0.8	7
119	A photo-induced excited state structure of a hetero-bimetallic ionic pair complex, Nd(DMA)4(H2O)4Fe(CN)6□3H2O, analyzed by single crystal X-ray diffraction. *Chemical Communications*, **2011**, 47, 9486-8	5.8	7
118	A Crystalline Microporous Narrow-Bandgap Semiconductor. *Angewandte Chemie*, **2004**, 116, 718-722	3.6	7
117	Group 13 Precursor Structures and Their Effect on Oxide Nanocrystal Formation. *Chemistry - A European Journal*, **2020**, 26, 1022-1026	4.8	7
116	Exploration of Phase Compositions, Crystal Structures, and Electrochemical Properties of NaxFeyMn1□yO2 Sodium Ion Battery Materials. *Chemistry of Materials*, **2018**, 30, 6636-6645	9.6	7
115	Supercritical Flow Synthesis of Pt1□Rux Nanoparticles: Comparative Phase Diagram Study of Nanostructure versus Bulk. *Chemistry of Materials*, **2017**, 29, 3265-3273	9.6	6
114	Magnetic correlations and structure in bixbyite across the spin-glass transition. *Physical Review B*, **2019**, 100,	3.3	6
113	Investigation of an Unusual Crystal Habit of Hydrochlorothiazide Reveals Large Polar Enantiopure Domains and a Possible Crystal Nucleation Mechanism. *Angewandte Chemie - International Edition*, **2019**, 58, 10255-10259	16.4	6
112	Low-Temperature Structural Phase Transitions in Thermoelectric Tetrahedrite, Cu12Sb4S13, and Tennantite, Cu12As4S13. *Crystal Growth and Design*, **2019**, 19, 3979-3988	3.5	6
111	Maximizing the Catalytically Active {001} Facets on Anatase Nanoparticles. *Chemistry of Materials*, **2020**, 32, 5134-5141	9.6	6
110	Is SrZn2Sb2 a Realistic Candidate for High-Temperature Thermoelectric Applications?. *Journal of Physical Chemistry C*, **2018**, 122, 5317-5324	3.8	6
109	Hydrothermal Synthesis of TiO2@SnO2 Hybrid Nanoparticles in a Continuous-Flow Dual-Stage Reactor. *ChemSusChem*, **2016**, 9, 532-9	8.3	6
108	Influence of Phase Separation and Spinodal Decomposition on Microstructure of Mg2Si1□Snx Alloys. *Crystal Growth and Design*, **2019**, 19, 4927-4933	3.5	6

107	Anisotropic thermal expansion in a metal-organic framework. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2014**, 70, 595-601	1.8	6
106	Kinetics, Stability, and Thermal Contact Resistance of Nickel□a3Co4O9 Interfaces Formed by Spark Plasma Sintering. *Journal of Electronic Materials*, **2013**, 42, 1661-1668	1.9	6
105	Thermal Instability of □Zn4Sb3: Insights from Transport and Structural Measurements. *Journal of Electronic Materials*, **2013**, 42, 1988-1991	1.9	6
104	High-pressure Single-crystal X-ray Diffraction Study of the Photomagnetic Switching Complex □ [Y(DMF)4(H2O)3(□CN)Fe(CN)5]□H2O. *Journal of the Chinese Chemical Society*, **2013**, 60, 929-934	1.5	6
103	Experimental Investigation of Zinc Antimonide Thin Film Thermoelectric Element over Wide Range of Operating Conditions. *Physica Status Solidi (A) Applications and Materials Science*, **2017**, 214, 1700301	1.6	6
102	Understanding the Reorientational Dynamics of Solid-State MBH4 (M = Li□s). *Journal of Physical Chemistry C*, **2015**, 119, 12109-12118	3.8	6
101	Electron□phonon coupling in the two-dimensional electron gas on Bi2Se3. *Physica Status Solidi - Rapid Research Letters*, **2013**, 7, 136-138	2.5	6
100	A High Temperature, High Pressure Facility for Controlled Studies of Catalytic Activity under Hydrothermal Conditions. *Energy & Fuels*, **2010**, 24, 2737-2746	4.1	6
99	Magnetic structure of Ni(DCOO)2(D2O)2. *Inorganic Chemistry*, **2011**, 50, 1441-6	5.1	6
98	Multipole electron densities and atomic displacement parameters in urea from accurate powder X-ray diffraction. *Acta Crystallographica Section A: Foundations and Advances*, **2019**, 75, 600-609	1.7	6
97	Effect of Mg-Doping on the Thermal Stability of Thermoelectric Zn4Sb3. *Science of Advanced Materials*, **2011**, 3, 592-595	2.3	6
96	Continuous flow hydrothermal synthesis of phase pure rutile TiO nanoparticles with a rod-like morphology. *Nanoscale*, **2020**, 12, 2695-2702	7.7	6
95	Selective Catalytic Reduction of NO Using Phase-Pure Anatase, Rutile, and Brookite TiO Nanocrystals. *Inorganic Chemistry*, **2020**, 59, 15324-15334	5.1	6
94	Facile synthesis of brookite TiO nanoparticles. *Chemical Communications*, **2020**, 56, 15084-15087	5.8	6
93	Temperature dependence of dynamic dipole formation in PbTe. *Physical Review B*, **2020**, 102,	3.3	6
92	Chemical Bonding Origin of the Thermoelectric Power Factor in Half-Heusler Semiconductors. *Chemistry of Materials*, **2021**, 33, 5308-5316	9.6	6
91	Continuous Flow Supercritical Water Synthesis and Temperature-Dependent Defect Structure Analysis of YAG and YbAG Nanoparticles. *Crystal Growth and Design*, **2016**, 16, 2646-2652	3.5	6
90	Operando powder X-ray diffraction study of P2-Na x Ni0.3Mn0.7O2 cathode material during electrochemical cycling. *Journal of Applied Crystallography*, **2018**, 51, 1304-1310	3.8	6

89	Structural Evolution during Lithium- and Magnesium-Ion Intercalation in Vanadium Oxide Nanotube Electrodes for Battery Applications. *ACS Applied Nano Materials*, **2018**, 1, 5071-5082	5.6	6
88	Pulsed laser deposition growth of FeSb2 films for thermoelectric applications. *Materials Chemistry and Physics*, **2011**, 129, 105-108	4.4	5
87	Crystal Structures and Physical Properties of Three New Manganese-Based Coordination Polymers with p-Biphenyldicarboxylic Acid Linkers. *European Journal of Inorganic Chemistry*, **2011**, 2011, 549-555	2.3	5
86	Electro-migration of Zinc during current-assisted pressure sintering of Zn4Sb3 Effect of process parameters and its influence on the thermoelectric properties. *Materials Research Society Symposia Proceedings*, **2011**, 1325, 137		5
85	Low-Temperature Synchrotron Radiation Study of a Twinned Disordered Crystal of Bis(4,4'-bromophenyl)-61,61-diyl Methano Fullerene C60. *Acta Crystallographica Section B: Structural Science*, **1998**, 54, 174-179		5
84	Tetraaquatetrakis(dimethylacetamide-O)neodymium(III) hexacyanoferrate(III) trihydrate. *Acta Crystallographica Section E: Structure Reports Online*, **2005**, 61, m268-m270		5
83	Starke NH???O-Wasserstoffbrücken bindungen in einer Modellverbindung für die katalytische Triade in Serinproteasen. *Angewandte Chemie*, **1999**, 111, 1321-1324	3.6	5
82	The Nature of Chemical Interactions in Anhydrous Sodalites, M6(AlSiO4)6, M = Na, Ag, Tl. *Chemistry of Materials*, **1999**, 11, 2912-2918	9.6	5
81	X-ray scattering study of thermoelectric ZnSb. *IUCrJ*, **2020**, 7, 100-104	4.7	5
80	Probing the validity of the spinel inversion model: a combined SPXRD, PDF, EXAFS and NMR study of ZnAlO. *Dalton Transactions*, **2020**, 49, 13449-13461	4.3	5
79	Autocatalytic Formation of High-Entropy Alloy Nanoparticles. *Angewandte Chemie*, **2020**, 132, 22104-22108	3.6	5
78	Multipole electron densities and structural parameters from synchrotron powder X-ray diffraction data obtained with a MYTHEN detector system (OHGI). *Acta Crystallographica Section A: Foundations and Advances*, **2021**, 77, 85-95	1.7	5
77	Low-Temperature Anharmonicity in Cesium Chloride (CsCl). *Angewandte Chemie*, **2017**, 129, 3679-3683	3.6	4
76	Why Does BiWO Visible-Light Photocatalyst Always Form as Nanoplatelets?. *Inorganic Chemistry*, **2020**, 59, 9364-9373	5.1	4
75	Mapping the redox chemistry of common solvents in solvothermal synthesis through in situ X-ray diffraction. *Nanoscale*, **2020**, 12, 8511-8518	7.7	4
74	Solvothermal flow synthesis of zinc phosphate pigment. *Dalton Transactions*, **2018**, 47, 9136-9142	4.3	4
73	Maximum Entropy Method Visualization of Disorder and Ion Migration in Thermoelectric Cu2-Se. *Advanced Theory and Simulations*, **2018**, 1, 1800068	3.5	4
72	Charakterisierung eines Mehrkomponenten-Lithiumlithats durch eine Kombination von Röntgenstrukturanalyse, NMR-Spektroskopie und theoretischen Studien. *Angewandte Chemie*, **2014**, 126, 13498-13503	3.6	4

71	Pushing X-ray Electron Densities to the Limit: Thermoelectric CoSb3. *Angewandte Chemie*, **2013**, 125, 1543-1546	3.6	4
70	Mössbauer spectroscopy study of defects in hydrothermally synthesized LiFePO4 cathode material. *Hyperfine Interactions*, **2014**, 226, 73-78	0.8	4
69	Rapid One-Step Low-Temperature Synthesis of Nanocrystalline α-Al2O3. *Angewandte Chemie*, **2011**, 123, 7183-7185	3.6	4
68	A gadolinium-based metal–organic framework, poly[[tris(μ4-benzene-1,4-dicarboxylato)bis(μ2-N,N-diethylformamide)digadolinium(III)] monohydrate]. *Acta Crystallographica Section E: Structure Reports Online*, **2005**, 61, m1337-m1339		4
67	Poly[sesqui(μ4-biphenyl-4,4′-dicarboxylato-κ4O:O′:O″:O‴)(diethylformamide-κO)gadolinium]. *Acta Crystallographica Section E: Structure Reports Online*, **2005**, 61, m2308-m2310		4
66	Three-dimensional morphology of anatase nanocrystals obtained from supercritical flow synthesis with industrial grade TiOSO precursor. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2019**, 75, 1086-1095	1.8	4
65	Direct observation of one-dimensional disordered diffusion channel in a chain-like thermoelectric with ultralow thermal conductivity. *Nature Communications*, **2021**, 12, 6709	17.4	4
64	Synchrotron total-scattering data applicable to dual-space structural analysis. *IUCrJ*, **2021**, 8, 387-394	4.7	4
63	Phase control for indium oxide nanoparticles. *Nanoscale*, **2021**, 13, 4038-4050	7.7	4
62	Charge Density Methods in Hydrogen Bond Studies **2010**, 53		4
61	Neutron and X-ray investigations of the Jahn–Teller switch in partially deuterated ammonium copper Tutton salt, (NH4)2[Cu(H2O)6](SO4)2. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2017**, 73, 87-93	1.8	3
60	Investigation of an Unusual Crystal Habit of Hydrochlorothiazide Reveals Large Polar Enantiopure Domains and a Possible Crystal Nucleation Mechanism. *Angewandte Chemie*, **2019**, 131, 10361-10365	3.6	3
59	The hydrothermal synthesis, crystal structure and electrochemical properties of MnSbO. *Dalton Transactions*, **2016**, 45, 18994-19001	4.3	3
58	Triaquatetrakis(dimethylacetamide-κO)gadolinium(III) hexacyanoferrate(III) dihydrate. *Acta Crystallographica Section E: Structure Reports Online*, **2006**, 62, m989-m991		3
57	An Eu-based metal–organic framework: poly[[tris(μ4-benzene-1,4-dicarboxylato)bis(μ2-N,N-diethylformamide)dieuropium(III)] 0.7-hydrate]. *Acta Crystallographica Section E: Structure Reports Online*, **2006**, 62, m3333-m3335		3
56	Bis(μ-diacetylacetonato)bis[pyridinecopper(II)]. *Acta Crystallographica Section E: Structure Reports Online*, **2005**, 61, m922-m924		3
55	A Novel Nanocomposite Material for Optically Stimulated Luminescence Dosimetry.. *Nano Letters*, **2022**,	11.5	3
54	Pair distribution function and Ga NMR study of aqueous Ga complexes. *Chemical Science*, **2021**, 12, 14420-14431	9.4	3

53	Improving Upconversion Efficiency by Photon Management in Self-Assembled Core/Shell Nanocrystal Films. *Journal of Physical Chemistry C*, **2020**, 124, 22357-22365	3.8	3
52	Anharmonicity and correlated dynamics of PbTe and PbS studied by single crystal x-ray scattering. *Physical Review B*, **2021**, 103,	3.3	3
51	X-Ray Diffraction and Mössbauer Spectroscopy Studies of Pressure-Induced Phase Transitions in a Mixed-Valence Trinuclear Iron Complex. *Chemistry - A European Journal*, **2016**, 22, 9616-23	4.8	3
50	Energy Harvesting from a Thermoelectric Zinc Antimonide Thin Film under Steady and Unsteady Operating Conditions. *Materials*, **2018**, 11,	3.5	3
49	Variable-temperature structural studies on valence tautomerism in cobalt bis(dioxolene) molecular complexes. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2017**, 73, 304-312	1.8	2
48	Single-Crystal High-Pressure X-ray Diffraction Study of Host Structure Compression in Clathrates of Dianin's Compound. *Crystal Growth and Design*, **2020**, 20, 4092-4099	3.5	2
47	Is RuAs a candidate for high temperature thermoelectric applications?. *Physical Chemistry Chemical Physics*, **2018**, 20, 9930-9937	3.6	2
46	High-pressure single crystal X-ray diffraction study of thermoelectric ZnSb and Zn4Sb. *Dalton Transactions*, **2016**, 45, 15097-15103	4.3	2
45	Electronic structure in FeSb2, FeAs2 and FeSi **2006**,		2
44	High Temperature stability of thermoelectric Zn4Sb3 **2006**,		2
43	Thermoelectric properties of nano-grained CoSb/sub 3/ skutterudites doped with Ni and Te		2
42	Thermoelectric performance of large single crystal clathrate Ba/sub 8/Ga/sub 16/Ge/sub 30/		2
41	Thermoelectric properties of hole doped FeSb/sub 2/ **2005**,		2
40	Rapid One-Step Synthesis and Compaction of High-Performance n-Type Mg3Sb2 Thermoelectrics. *Angewandte Chemie*, **2020**, 132, 4308-4312	3.6	2
39	Zinc antimonide thin film based flexible thermoelectric module. *Materials Letters*, **2020**, 280, 128582	3.3	2
38	Bandgap Tuning in Molecular Alloy Crystals Formed by Weak Chalcogen Interactions. *Journal of Physical Chemistry Letters*, **2021**, 12, 3059-3065	6.4	2
37	Tuneable local order in thermoelectric crystals. *IUCrJ*, **2021**, 8, 695-702	4.7	2
36	Sample dependent performance of aqueous copper hexacyanoferrate/zinc batteries. *Materials Advances*, **2021**, 2, 2036-2044	3.3	2

35	Transport properties and crystal structure of layered LaSb2. *Journal of Applied Physics*, **2019**, 125, 045110	2.5	1
34	Evolution of the Polymorph Selectivity of Titania Formation under Acidic and Low-Temperature Conditions. *ACS Omega*, **2019**, 4, 5750-5757	3.9	1
33	Chemical Bonding in Colossal Thermopower FeSb. *Chemistry - A European Journal*, **2020**, 26, 8651-8662	4.8	1
32	trans-Dibromidobis(1-ethyl-3-methyl-imidazol-2-yl-idene)palladium(II). *Acta Crystallographica Section E: Structure Reports Online*, **2011**, 67, m1205		1
31	Particle size effects on the thermal conductivity of ZnO **2012**,		1
30	An exploration of noble metal substitution in germanium based clathrates **2007**,		1
29	Standardisation in thermoelectric transport properties measurements - the Cardiff NEDO laboratories and DLR Cologne program		1
28	Theoretical modeling of Te doped CoSb/sub 3/		1
27	Copper containing germanium clathrates **2005**,		1
26	Magnetic Structure and Thermal Expansion of Eu4Ga8Ge16. *Materials Research Society Symposia Proceedings*, **2002**, 755, 1		1
25	Synthesis and structural characterization of AI2O3 nanoparticles: Towards 3D optically stimulated luminescence dosimetry. *Journal of Physics: Conference Series*, **2022**, 2167, 012023	0.3	1
24	Exciting Opportunities for Solid-State Mo NMR Studies of MoS Nano-structures in Materials Research from Low to Ultra-high Magnetic Field (35.2 T). *Journal of Physical Chemistry C*, **2021**, 125, 7824-7838	3.8	1
23	Insights into Host□Guest Binding in Hydroquinone Clathrates: Single-Crystal X-ray and Neutron Diffraction, and Complementary Computational Studies on the Hydroquinone-CO2 Clathrate. *Crystal Growth and Design*, **2021**, 21, 3477-3486	3.5	1
22	Operando structural investigations of thermoelectric materials. *Journal of Applied Crystallography*, **2021**, 54, 1189-1197	3.8	1
21	Procrystal analysis as a tool for the visualization of ion migration pathways **2016**,		1
20	Accessing the rich carbon nitride materials chemistry by heat treatments of ammonium thiocyanate, NHSCN. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2019**, 75, 621-633	1.8	1
19	Tailoring the stoichiometry of CN nanosheets under electron beam irradiation. *Physical Chemistry Chemical Physics*, **2021**, 23, 4747-4756	3.6	1
18	Unravelling the complex formation mechanism of HfO nanocrystals using in situ pair distribution function analysis. *Nanoscale*, **2021**, 13, 12711-12719	7.7	1

17	Stability and Thermoelectric Properties of ZnSb with TiO Nanoparticle Inclusions. *ACS Applied Materials & Interfaces*, **2021**, 13, 45708-45716	9.5	1
16	On single-crystal total scattering data reduction and correction protocols for analysis in direct space. *Acta Crystallographica Section A: Foundations and Advances*, **2021**, 77, 611-636	1.7	0
15	Structural evolution in thermoelectric zinc antimonide thin films studied by X-ray scattering techniques. *IUCrJ*, **2021**, 8, 444-454	4.7	0
14	Tuning of bandgaps and emission properties of light-emitting diode materials through homogeneous alloying in molecular crystals. *Chemical Science*, **2021**, 12, 12391-12399	9.4	0
13	Strongly Correlated Intermetallics: (mathbf FeSb _mathbf{2}). *Springer Series in Materials Science*, **2013**, 71-93	0.9	
12	Charge Density in Materials and Energy Science **2011**, 469-504		
11	Time Induced Changes in Phase Transition Behavior and Stability of Zn4Sb3. *Materials Research Society Symposia Proceedings*, **2006**, 945, 1		
10	Hexaaqua-1κ O,3κ O-tri-μ-cyano-1:2κ N:C;2:3κ C:N;3:4κ N:C-nonacyano-2κ C,4κ C-pentakis(N,N-dimethylacetamide)-1κ O,3κ O-diiron(III)diytterbium(III) dihydrate. *Acta Crystallographica Section E: Structure Reports Online*, **2006**, 62, m793-m795		
9	Nuclear Density Analysis in Solids. The Case of Ba8Ga16Si30. *Materials Research Society Symposia Proceedings*, **2001**, 691, 1		
8	Maximum Entropy Method Charge Density Distributions of Novel Thermoelectric Clathrates. *Materials Research Society Symposia Proceedings*, **1999**, 590, 145		
7	Charge Transfer and Local Structure in Thermoelectric Germanium Clathrates. *Materials Research Society Symposia Proceedings*, **1999**, 590, 51		
6	Two structures involved in the separation of the enantiomeric pair of 2,2'-spirobi[indan]-1,1'-dione. *Acta Crystallographica Section C: Crystal Structure Communications*, **1993**, 49, 1104-1107		
5	Effects of Voigt diffraction peak profiles on the pair distribution function.. *Acta Crystallographica Section A: Foundations and Advances*, **2022**, 78, 10-20	1.7	
4	Reliability of charge density distributions derived by the maximum entropy method **2000**, 27-36		
3	The Structure of High-performance Thermoelectric Material, .BETA.-Zn4Sb3 by Maximum Entropy Method. *Nihon Kessho Gakkaishi*, **2005**, 47, 204-210	0	
2	Structural Studies of Thermoelectric Materials **2005**, 21-1-21-19		
1	Locating Fe dopants in catalytic PtPd nanoparticles on γ-alumina using X-ray absorption spectroscopy. *Catalysis Science and Technology*, **2021**, 11, 1961-1964	5.5	