

# Antti J Karttunen

## List of Publications by Year in Descending Order

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

200  
papers

3,219  
citations

30  
h-index

45  
g-index

232  
ext. papers

3,640  
ext. citations

4.9  
avg, IF

5.56  
L-index

#	Paper	IF	Citations
200	Chemi-Inspired Silicon Allotropes-Experimentally Accessible Si Cages as Proposed Building Block for 1D Polymers, 2D Sheets, Single-Walled Nanotubes, and Nanoparticles.. <i>Molecules</i> , <b>2022</b> , 27,	4.8	1
199	Surprises in the Solvent-Induced Self-Ionization in the Uranium Tetrahalide UX (X = Cl, Br, I)/Ethyl Acetate System.. <i>ACS Omega</i> , <b>2022</b> , 7, 11995-12003	3.9	
198	VRChem: A Virtual Reality Molecular Builder. <i>Applied Sciences (Switzerland)</i> , <b>2021</b> , 11, 10767	2.6	1
197	DFT-Guided Crystal Structure Redetermination and Lattice Dynamics of the Intermetallic Actinoid Compound UIr. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 16686-16699	5.1	
196	Coexistence of Two Different Distorted Octahedral [MnF] Sites in K [MnF]: Manifestation in Spectroscopy and Magnetism. <i>Chemistry - A European Journal</i> , <b>2021</b> , 27, 9801-9813	4.8	5
195	Aliovalent substitution in phosphide-based materials [Crystal structures of Na <sub>10</sub> AlTaP <sub>6</sub> and Na <sub>3</sub> GaP <sub>2</sub> featuring edge-sharing EP <sub>4</sub> tetrahedra (E=Al/Ta and Ga). <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2021</b> , 647, 1804-1814	1.3	
194	Reactions of ThX <sub>4</sub> (X=F, Cl, Br, I) with Liquid Ammonia-Crystal Structures and a Theoretical Study of Ammine Thorium(IV) Halide Ammoniates. <i>European Journal of Inorganic Chemistry</i> , <b>2021</b> , 2021, 2787-2796 <sup>2,3</sup>	2.3	0
193	Photochemical Synthesis of Tungsten Pentafluoride, WF <sub>5</sub> . <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2021</b> , 647, 218-224	1.3	3
192	Boranyl-Functionalized [Ge] Clusters: Providing the Idea of Intramolecular Ge/B Frustrated Lewis Pairs. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 2648-2653	16.4	13
191	Boranyl-Functionalized [Ge <sub>9</sub> ] Clusters: Providing the Idea of Intramolecular Ge/B Frustrated Lewis Pairs. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 2680-2685	3.6	3
190	Photochemistry with Chlorine Trifluoride: Syntheses and Characterization of Difluoroxychloronium(V) Hexafluorido(non)metallates(V), [ClOF][MF] (M=V, Nb, Ta, Ru, Os, Ir, P, Sb). <i>Chemistry - A European Journal</i> , <b>2021</b> , 27, 2381-2392	4.8	1
189	Learning experiences from digital laboratory safety training. <i>Education for Chemical Engineers</i> , <b>2021</b> , 34, 87-93	2.4	7
188	Emergence of Metallic Conductivity in Ordered One-Dimensional Coordination Polymer Thin Films upon Reductive Doping. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2021</b> , 13, 10249-10256	9.5	2
187	Na <sub>3</sub> SO <sub>4</sub> H Ein erster Vertreter der Materialklasse der Sulfathydride. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 5747-5751	3.6	0
186	Na SO H-The First Representative of the Material Class of Sulfate Hydrides. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 5683-5687	16.4	4
185	A Comprehensive Study on the Full Series of Alkali-Metal Selenocyanates A [SeCN] (A =Li-Cs). <i>Chemistry - A European Journal</i> , <b>2021</b> , 27, 13552-13557	4.8	5
184	Syntheses and Characterization of the Mixed-Valent Manganese(II/III) Fluorides MnF and MnF. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 12651-12663	5.1	

183	Reactions of [SiF(NH)] with Fluorides AF (A = Li-Cs, Tl, NH) in Liquid NH: A [NH(NH)] Cation and a Thallophilic Interaction in [Tl(NH)]. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 15031-15040	5.1	
182	Mn(IV)-Substituted Metal(II) Hexafluorido Metallates(IV): Synthesis, Crystal Structures, and Luminescence Properties. <i>European Journal of Inorganic Chemistry</i> , <b>2021</b> , 2021, 3861	2.3	0
181	Reactions of ClF <sub>3</sub> with Main Group and Transition Metal Oxides: Access to Dioxychloronium(V) Fluoridometallates and Oxidofluoridometallates. <i>European Journal of Inorganic Chemistry</i> , <b>2021</b> , 2021, 405-421	2.3	3
180	Probing lattice dynamics in ST 12 phase germanium nanowires by Raman spectroscopy. <i>Applied Physics Letters</i> , <b>2021</b> , 119, 232105	3.4	0
179	The Crystal Structure of MnF <sub>3</sub> Revisited. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2020</b> , 646, 882-888	1.3	2
178	Speciation of Be in acidic liquid ammonia and formation of tetra- and octanuclear beryllium amido clusters. <i>Chemical Science</i> , <b>2020</b> , 11, 5415-5422	9.4	9
177	Electronic band structures of pristine and chemically modified cellulose allomorphs. <i>Carbohydrate Polymers</i> , <b>2020</b> , 243, 116440	10.3	5
176	Toward Atomic-Scale Inorganic Double Helices via Carbon Nanotube Matrices Induction of Chirality to Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 13338-13347	3.8	4
175	Borate Hydrides as a New Material Class: Structure, Computational Studies, and Spectroscopic Investigations on Sr (BO) <sub>2</sub> H and Sr (BO) <sub>2</sub> D. <i>Chemistry - A European Journal</i> , <b>2020</b> , 26, 11742-11750	4.8	5
174	Cs[Cl F]: A Propeller-Shaped [Cl F] Anion in a Peculiar A B Structure Type. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 18116-18119	16.4	2
173	Cs[Cl <sub>3</sub> F <sub>10</sub> ]: Eine Verbindung mit propellerförmigem [Cl <sub>3</sub> F <sub>10</sub> ] Anion, die im außergewöhnlichen A[5]B[5]-Strukturtyp kristallisiert. <i>Angewandte Chemie</i> , <b>2020</b> , 132, 18272-18276	3.6	0
172	Key Role of Defects in Thermoelectric Performance of TiMSn (M = Ni, Pd, and Pt) Half-Heusler Alloys. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 14997-15006	3.8	8
171	Synthesis and Characterization of the Tetrafluoridochlorates(III) A[ClF <sub>4</sub> ] (A = K, Rb, Cs). <i>European Journal of Inorganic Chemistry</i> , <b>2020</b> , 2020, 1319-1324	2.3	6
170	Atomic/molecular layer deposition and electrochemical performance of dilithium 2-aminoterephthalate. <i>Dalton Transactions</i> , <b>2020</b> , 49, 1591-1599	4.3	13
169	Evolutionary Algorithm-based Crystal Structure Prediction for Gold(I) Fluoride. <i>ChemPhysChem</i> , <b>2020</b> , 21, 802-808	3.2	4
168	Synthesis and Characterization of A[W <sub>2</sub> O <sub>2</sub> F <sub>9</sub> ] (A = Li [Cs]). <i>European Journal of Inorganic Chemistry</i> , <b>2020</b> , 2020, 2260-2269	2.3	3
167	Difluorochloronium(III) Fluoridometallates From Molecular Building Blocks to (Helical) Chains. <i>European Journal of Inorganic Chemistry</i> , <b>2020</b> , 2020, 4483-4496	2.3	0
166	Preparation of Two Quantum-Chemically Predicted, Isomeric [Br <sub>4</sub> F <sub>13</sub> ] Anions in the Solid State. <i>European Journal of Inorganic Chemistry</i> , <b>2020</b> , 2020, 4568-4576	2.3	

165	A brief visit to the BeCl <sub>2</sub> /ZnCl <sub>2</sub> system and the prediction of a new polymorph of ZnCl <sub>2</sub> . <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , <b>2020</b> , 75, 491-496	1	
164	FeSe: a possible ferrimagnetic half-metal?. <i>Journal of Physics Condensed Matter</i> , <b>2020</b> , 32, 455801	1.8	0
163	Compressive Properties of Micro-spherical SiO <sub>2</sub> Particles. <i>Minerals, Metals and Materials Series</i> , <b>2020</b> , 57-66	0.3	
162	Lattice thermal conductivity of NaCoO <sub>2</sub> and LiCoO <sub>2</sub> intercalation materials studied by hybrid density functional theory. <i>Materials Research Express</i> , <b>2020</b> , 7, 075502	1.7	5
161	PbF[Br <sub>2</sub> F <sub>7</sub> ], a Fluoridobromate(III) of a p-Block Metal. <i>European Journal of Inorganic Chemistry</i> , <b>2020</b> , 2020, 64-70	2.3	6
160	Rb <sub>2</sub> [U(NH <sub>2</sub> ) <sub>6</sub> ], a Rubidium Hexaamidouranate(IV) obtained from the Reaction of UI <sub>3</sub> with RbNH <sub>2</sub> in Anhydrous Ammonia. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2020</b> , 646, 1023-1029	1.3	0
159	Reactions in Anhydrous Liquid Ammonia: Syntheses and Crystal Structures of [M(NH <sub>3</sub> ) <sub>8</sub> ]I <sub>2</sub> (M = Eu, Yb) with Bicapped Trigonal-Prismatic Octaammine Lanthanoid(II) Cations. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2020</b> , 646, 1396-1402	1.3	
158	Complexes featuring a linear [N?U?N] core isoelectronic to the uranyl cation. <i>Nature Chemistry</i> , <b>2020</b> , 12, 962-967	17.6	13
157	A recycling process for thermoelectric devices developed with the support of statistical entropy analysis. <i>Resources, Conservation and Recycling</i> , <b>2020</b> , 159, 104843	11.9	3
156	Binary Lead Fluoride Pb F. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 15656-15661	4.8	2
155	Crystal Structures of $\text{U}^{\text{IV}}$ and $\text{N}^{\text{III}}$ Nitrogen Trifluoride. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 6422-6430	5.1	1
154	A Revised Structure Model for the UCl Structure Type, Novel Modifications of UCl and UBr, and a Comment on the Modifications of Protactinium Pentabromides. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 6402-6411	4.8	4
153	UF and the High-Pressure Polymorph HP-UF. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 7366-7374	4.8	
152	Synthesis and Characterization of [Br][MF] (M=Sb, Ir), as well as Quantum Chemical Study of [Br] Structure, Chemical Bonding, and Relativistic Effects Compared with [XBr] (X=Br, I, At, Ts) and [TsZ] (Z=F, Cl, Br, I, At, Ts). <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 5793-5802	4.8	7
151	Silicon clusters with six and seven unsubstituted vertices a two-step reaction from elemental silicon. <i>Chemical Science</i> , <b>2019</b> , 10, 9130-9139	9.4	8
150	Lewis Acidic Behavior of MoOF <sub>4</sub> towards the Alkali Metal Fluorides in Anhydrous Hydrogen Fluoride Solutions. <i>European Journal of Inorganic Chemistry</i> , <b>2019</b> , 2019, 3672-3682	2.3	8
149	Evolutionary Algorithm-Based Crystal Structure Prediction for Copper(I) Fluoride. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 11528-11537	4.8	4
148	A Facile Molecular Machine: Optically Triggered Counterion Migration by Charge Transfer of Linear Donor-Acceptor Phosphonium Fluorophores. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 13590-13599	3.6	7

147	A Facile Molecular Machine: Optically Triggered Counterion Migration by Charge Transfer of Linear Donor-Acceptor Phosphonium Fluorophores. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 13456-13465	16.4	24
146	Lattice thermal conductivity of TiS <sub>2</sub> , ZrS <sub>2</sub> , and HfS <sub>2</sub> : Periodic trends studied by dispersion-corrected hybrid density functional methods. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	5
145	Lattice dynamical properties of antiferromagnetic MnO, CoO, and NiO, and the lattice thermal conductivity of NiO. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	6
144	An Unprecedented Fully H <sub>2</sub> Substituted Phosphate Hydride Sr <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> H Expanding the Apatite Family. <i>European Journal of Inorganic Chemistry</i> , <b>2019</b> , 2019, 5073-5076	2.3	8
143	Negative thermal expansion of CuO studied by quasi-harmonic approximation and cubic force-constant method. <i>Journal of Chemical Physics</i> , <b>2019</b> , 151, 184109	3.9	2
142	Half-metallicity in uranium intermetallics: crystal structure prediction of a high-pressure phase of UCo. <i>Journal of Physics Condensed Matter</i> , <b>2019</b> , 31, 025501	1.8	0
141	The Crystal Structures of H <sub>2</sub> and HF Revisited. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 3310-3317	4.8	2
140	Reactions of KBrF <sub>4</sub> with platinum metals. <i>Journal of Fluorine Chemistry</i> , <b>2019</b> , 218, 11-20	2.1	4
139	Supramolecular Construction of Cyanide-Bridged Re Diimine Multichromophores. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 1988-2000	5.1	6
138	F-bridged Anions of Bromine and Gold: Predictions of Unexpected Behavior. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2019</b> , 645, 284-291	1.3	6
137	Numerical study on the fluid dynamical aspects of atomic layer deposition process. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , <b>2018</b> , 36, 021516	2.9	10
136	The [U <sub>2</sub> F <sub>12</sub> ] <sup>2-</sup> Anion of Sr[U <sub>2</sub> F <sub>12</sub> ]. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 2964-2968	3.6	5
135	The [U F ] Anion of Sr[U F ]. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 2914-2918	16.4	9
134	Luminescence Thermochromism of Gold(I) Phosphane-Iodide Complexes: A Rule or an Exception?. <i>Chemistry - A European Journal</i> , <b>2018</b> , 24, 3021-3029	4.8	13
133	Thermoelectric applications for energy harvesting in domestic applications and micro-production units. Part I: Thermoelectric concepts, domestic boilers and biomass stoves. <i>Renewable and Sustainable Energy Reviews</i> , <b>2018</b> , 98, 519-544	16.2	14
132	On the Affinity between Fullerenes and Deltahedral Zintl Ions: A UV/Vis Spectroscopic Investigation. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2018</b> , 644, 1337-1343	1.3	2
131	On the exfoliation and anisotropic thermal expansion of black phosphorus. <i>Chemical Communications</i> , <b>2018</b> , 54, 9793-9796	5.8	11
130	Synthesis and Characterization of Barium Hexafluoridoosmates. <i>Crystals</i> , <b>2018</b> , 8, 11	2.3	4

- 129 Charged Si Clusters in Neat Solids and the Detection of [H Si ] in Solution: A Combined NMR, Raman, Mass Spectrometric, and Quantum Chemical Investigation. *Angewandte Chemie - International Edition*, **2018**, 57, 12950-12955 16.4 23
- 128 MoF5 revisited. A comprehensive study of MoF5. *Journal of Fluorine Chemistry*, **2018**, 211, 171-179 2.1 12
- 127 Charged Si<sub>9</sub> Clusters in Neat Solids and the Detection of [H<sub>2</sub>Si<sub>9</sub>]<sup>2+</sup> in Solution: A Combined NMR, Raman, Mass Spectrometric, and Quantum Chemical Investigation. *Angewandte Chemie*, **2018**, 130, 13132-13137 3.6 8
- 126 Improvement of the Photophysical Performance of Platinum-Cyclometalated Complexes in Halogen-Bonded Adducts. *Chemistry - A European Journal*, **2018**, 24, 11475-11484 4.8 25
- 125 Thermoelectric Properties of p-Type CuO, CuO, and NiO from Hybrid Density Functional Theory. *Journal of Physical Chemistry C*, **2018**, 122, 15180-15189 3.8 24
- 124 A Neutron Diffraction and Quantum-Chemical Study of [Mn(ND<sub>3</sub>)<sub>6</sub>](N<sub>3</sub>)<sub>2</sub>. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2018**, 644, 1349-1353 1.3
- 123 Die Interhalogenkationen [Br<sub>2</sub>F<sub>5</sub>]<sup>+</sup> und [Br<sub>3</sub>F<sub>8</sub>]<sup>+</sup>. *Angewandte Chemie*, **2018**, 130, 14850-14855 3.6 9
- 122 Electronic and Vibrational Properties of TiS<sub>2</sub>, ZrS<sub>2</sub>, and HfS<sub>2</sub>: Periodic Trends Studied by Dispersion-Corrected Hybrid Density Functional Methods. *Journal of Physical Chemistry C*, **2018**, 122, 26835-26844 3.8 21
- 121 The Fluoroperovskite TlMnF<sub>3</sub>. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2018**, 644, 1557-1561 1.3 0
- 120 Crystal Structure Prediction of Magnetic Transition-Metal Oxides by Using Evolutionary Algorithm and Hybrid DFT Methods. *Journal of Physical Chemistry C*, **2018**, 122, 24949-24957 3.8 10
- 119 Anionic Siliconoids from Zintl Phases: R Si with Six and R Si with Seven Unsubstituted Exposed Silicon Cluster Atoms (R=Si(tBu) H). *Chemistry - A European Journal*, **2018**, 24, 19171-19174 4.8 17
- 118 Heterometallic Cluster-Capped Tetrahedral Assemblies with Postsynthetic Modification of the Metal Cores. *Angewandte Chemie*, **2018**, 130, 14350-14354 3.6 3
- 117 Heterometallic Cluster-Capped Tetrahedral Assemblies with Postsynthetic Modification of the Metal Cores. *Angewandte Chemie - International Edition*, **2018**, 57, 14154-14158 16.4 23
- 116 Synthesis and characterization of the pyridineBromine trifluoride (1/1) complex, [pyBrF<sub>3</sub>]. *Journal of Fluorine Chemistry*, **2018**, 215, 17-24 2.1 5
- 115 The Interhalogen Cations [Br F ] and [Br F ]. *Angewandte Chemie - International Edition*, **2018**, 57, 14640-14644 16.4 11
- 114 Silver Alkynyl-Phosphine Clusters: An Electronic Effect of the Alkynes Defines Structural Diversity. *Organometallics*, **2017**, 36, 480-489 3.8 21
- 113 Dispersion interactions in silicon allotropes. *Physical Chemistry Chemical Physics*, **2017**, 19, 7699-7707 3.6 5
- 112 Lithium Aryloxide Thin Films with Guest-Induced Structural Transformation by ALD/MLD. *Chemistry - A European Journal*, **2017**, 23, 2988-2992 4.8 22

111	Exfoliation Energy of Black Phosphorus Revisited: A Coupled Cluster Benchmark. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 1290-1294	6.4	26
110	Dibenzothiophene-platinated complexes: probing the effect of ancillary ligands on the photophysical performance. <i>Dalton Transactions</i> , <b>2017</b> , 46, 3895-3905	4.3	13
109	Flexible Thermoelectric ZnO/Organic Superlattices on Cotton Textile Substrates by ALD/MLD. <i>Advanced Electronic Materials</i> , <b>2017</b> , 3, 1600459	6.4	37
108	Slicing Diamond for More sp Group 14 Allotropes Ranging from Direct Bandgaps to Poor Metals. <i>ChemPhysChem</i> , <b>2017</b> , 18, 1992-2006	3.2	5
107	Atomic Layer Deposition of Thermoelectric Materials <b>2017</b> , 259-274		
106	Cyclometalated Platinum(II) Cyanometallates: Luminescent Blocks for Coordination Self-Assembly. <i>Inorganic Chemistry</i> , <b>2017</b> , 56, 4460-4468	5.1	26
105	Slicing Diamond-A Guide to Deriving sp <sup>-</sup> Si Allotropes. <i>Chemistry - A European Journal</i> , <b>2017</b> , 23, 2734-2747	4.78	15
104	Syntheses and Crystal Structures of Sodium Hydrogen Fluorides NaF <sub>n</sub> HF (n = 2, 3, 4). <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2017</b> , 643, 1436-1443	1.3	7
103	The Cross-section of a Multi-disciplinary Project in View of Smart Textile Design Practice. <i>Journal of Textile Design Research and Practice</i> , <b>2017</b> , 5, 175-207	0.1	3
102	One-Dimensional Phosphorus Nanostructures: from Nanorings to Nanohelices. <i>Chemistry - A European Journal</i> , <b>2017</b> , 23, 15884-15888	4.8	13
101	Copper-mediated phospho-annulation to attain water-soluble polycyclic luminophores. <i>Chemical Communications</i> , <b>2017</b> , 53, 10954-10957	5.8	17
100	Ab initio study of the lattice thermal conductivity of Cu <sub>2</sub> O using the generalized gradient approximation and hybrid density functional methods. <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	31
99	Slicing Diamond for More sp <sup>3</sup> Group 14 Allotropes Ranging from Direct Bandgaps to Poor Metals. <i>ChemPhysChem</i> , <b>2017</b> , 18, 1960-1960	3.2	
98	A 1D Coordination Polymer of UF with HCN as a Ligand. <i>Chemistry - A European Journal</i> , <b>2017</b> , 23, 291-295	5.8	8
97	Ab initio studies on the lattice thermal conductivity of silicon clathrate frameworks II and VIII. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	10
96	NOUF <sub>6</sub> Revisited: A Comprehensive Study of a Hexafluoridouranate(V) Salt. <i>Chemistry - A European Journal</i> , <b>2016</b> , 22, 12145-53	4.8	9
95	[Ge <sub>2</sub> ] <sub>4</sub> Dumbbells with Very Short Ge-Ge Distances in the Zintl Phase Li <sub>3</sub> NaGe <sub>2</sub> : A Solid-State Equivalent to Molecular O <sub>2</sub> . <i>Angewandte Chemie</i> , <b>2016</b> , 128, 1087-1091	3.6	7
94	Harnessing Fluorescence versus Phosphorescence Ratio via Ancillary Ligand Fine-Tuned MLCT Contribution. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 12196-12206	3.8	22

93	Toward an Accurate Estimate of the Exfoliation Energy of Black Phosphorus: A Periodic Quantum Chemical Approach. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 131-6	6.4	46
92	Luminescent Triphosphine Cyanide d(10) Metal Complexes. <i>Inorganic Chemistry</i> , <b>2016</b> , 55, 2174-84	5.1	36
91	Layer-by-layer design of nanostructured thermoelectrics: First-principles study of ZnO:organic superlattices fabricated by ALD/MLD. <i>Nano Energy</i> , <b>2016</b> , 22, 338-348	17.1	24
90	[Ge <sub>2</sub> ](4-) Dumbbells with Very Short Ge-Ge Distances in the Zintl Phase Li <sub>3</sub> NaGe <sub>2</sub> : A Solid-State Equivalent to Molecular O <sub>2</sub> . <i>Angewandte Chemie - International Edition</i> , <b>2016</b> , 55, 1075-9	16.4	12
89	Ab initio computational study on the lattice thermal conductivity of Zintl clathrates [Si <sub>19</sub> P <sub>4</sub> ]Cl <sub>4</sub> and Na <sub>4</sub> [Al <sub>4</sub> Si <sub>19</sub> ]. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	5
88	Ambipolar Phosphine Derivatives to Attain True Blue OLEDs with 6.5% EQE. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2016</b> , 8, 10968-76	9.5	28
87	Substantially enhanced Raman signal for inorganic-organic nanocomposites by ALD-TiO <sub>2</sub> capping. <i>RSC Advances</i> , <b>2016</b> , 6, 41087-41091	3.7	1
86	BrF and BrF: peculiar anions showing $\pi$ and $\sigma$ bridging F-atoms. <i>Chemical Communications</i> , <b>2016</b> , 52, 12040-12043	5.8	21
85	Alkynyl triphosphine copper complexes: synthesis and photophysical studies. <i>Dalton Transactions</i> , <b>2015</b> , 44, 13294-304	4.3	9
84	The reactions of TiCl <sub>3</sub> , and of UF <sub>4</sub> with TiCl <sub>3</sub> in liquid ammonia: unusual coordination spheres in [Ti(NH <sub>3</sub> ) <sub>8</sub> ]Cl <sub>3</sub> ·6NH <sub>3</sub> and [UF(NH <sub>3</sub> ) <sub>8</sub> ]Cl <sub>3</sub> ·5NH <sub>3</sub> . <i>Chemical Communications</i> , <b>2015</b> , 51, 11826-9	5.8	6
83	On copper(I) fluorides, the cuprophilic interaction, the preparation of copper nitride at room temperature, and the formation mechanism at elevated temperatures. <i>Chemistry - A European Journal</i> , <b>2015</b> , 21, 3290-303	4.8	29
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