Carlo Gatti

List of Publications by Year in Descending Order

145 papers	7,258 citations	45 h-index	83 g-index
173 ext. papers	7,870 ext. citations	5 avg, IF	5.97 L-index

#	Paper	IF	Citations
145	Unravelling functions of halogen substituents in the enantioseparation of halogenated planar chiral ferrocenes on polysaccharide-based chiral stationary phases: experimental and electrostatic potential analyses.. *Journal of Chromatography A*, **2022**, 1673, 463097	4.5	0
144	Computational Modeling of 2D Materials under High Pressure and Their Chemical Bonding: Silicene as Possible Field-Effect Transistor. *ACS Nano*, **2021**, 15, 6861-6871	16.7	5
143	Metal-Metal Bond in the Light of Pauling Rules. *Molecules*, **2021**, 26,	4.8	4
142	Enantioseparation of 5,5-Dibromo-2,2-Dichloro-3-Selanyl-4,4-Bipyridines on Polysaccharide-Based Chiral Stationary Phases: Exploring Chalcogen Bonds in Liquid-Phase Chromatography. *Molecules*, **2021**, 26,	4.8	6
141	Charge Density Analysis of Actinide Compounds from the Quantum Theory of Atoms in Molecules and Crystals. *Journal of Physical Chemistry Letters*, **2021**, 12, 1862-1868	6.4	4
140	A revisit of the bond valence model makes it universal. *Physical Chemistry Chemical Physics*, **2020**, 22, 13839-13849	3.6	5
139	A tool for deciphering the redox potential ranking of organic compounds: a case study of biomass-extracted quinones for sustainable energy. *Physical Chemistry Chemical Physics*, **2020**, 22, 20212-20226	3.6	9
138	Steric and Electrostatic Effects in Compounds with Centered Clusters Quantified by Bond Order Analysis. *Crystal Growth and Design*, **2020**, 20, 2115-2122	3.5	2
137	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
136	Looking at local classical and quantum forces in stable crystals using multipole-model refined electron densities and orbital-free DFT approximations. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2020**, 76, 724-726	1.8	1
135	Halogen bond in separation science: A critical analysis across experimental and theoretical results. *Journal of Chromatography A*, **2020**, 1616, 460788	4.5	13
134	Factors Impacting and Hole Regions as Revealed by the Electrostatic Potential and Its Source Function Reconstruction: The Case of 4,4-Bipyridine Derivatives. *Molecules*, **2020**, 25,	4.8	6
133	Spin Density Topology. *Molecules*, **2020**, 25,	4.8	9
132	Assessing the Strength of Metal-Metal Interactions. *Inorganic Chemistry*, **2019**, 58, 7466-7471	5.1	4
131	Nine questions on energy decomposition analysis. *Journal of Computational Chemistry*, **2019**, 40, 2248-2283	3.9	70
130	A Quantum-Mechanical Map for Bonding and Properties in Solids. *Advanced Materials*, **2019**, 31, e1806280	24	134
129	Quantum Crystallography: Current Developments and Future Perspectives. *Chemistry - A European Journal*, **2018**, 24, 10881-10905	4.8	77

128	An Electron Density Source-Function Study of DNA Base Pairs in Their Neutral and Ionized Ground States. *Journal of Computational Chemistry*, **2018**, 39, 1112-1128	3.5	10
127	Probing Cyclic Electron Delocalization in an Imidazol-2-ylidene and a Corresponding Imidazolium Salt. *Chemistry - A European Journal*, **2018**, 24, 4973-4981	4.8	7
126	Spin density accuracy and distribution in azido Cu(II) complexes: A source function analysis. *Journal of Computational Chemistry*, **2018**, 39, 587-603	3.5	8
125	Chapter 5:Chemical Bonding Investigations for Materials **2018**, 117-175		2
124	A variable-temperature X-ray diffraction and theoretical study of conformational polymorphism in a complex organic molecule (DTC).. *RSC Advances*, **2018**, 8, 38445-38454	3.7	7
123	Bond Order Conservation Principle and Peculiarities of the Metal-Metal Bonding. *Inorganic Chemistry*, **2018**, 57, 15550-15557	5.1	6
122	Do the basic crystal chemistry principles agree with a plethora of recent quantum chemistry data?. *IUCrJ*, **2018**, 5, 542-547	4.7	7
121	Enantioseparation of fluorinated 3-arylthio-4,4′-bipyridines: Insights into chalcogen and hole bonds in high-performance liquid chromatography. *Journal of Chromatography A*, **2018**, 1567, 119-129	4.5	16
120	A stable compound of helium and sodium at high pressure. *Nature Chemistry*, **2017**, 9, 440-445	17.6	199
119	High-Temperature Crystal Structure and Chemical Bonding in Thermoelectric Germanium Selenide (GeSe). *Chemistry - A European Journal*, **2017**, 23, 6888-6895	4.8	29
118	Insights on spin delocalization and spin polarization mechanisms in crystals of azido copper(II) dinuclear complexes through the electron spin density Source Function. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2017**, 73, 565-583	1.8	10
117	Electronic structure and energy decomposition analyses as a tool to interpret the redox potential ranking of naphtho-, biphenyl- and biphenylene-quinone isomers. *Physical Chemistry Chemical Physics*, **2016**, 18, 26651-26660	3.6	11
116	The role of exchange correlation functional on the description of multiferroic properties using density functional theory: the ATiO3 (A = Mn, Fe, Ni) case study. *RSC Advances*, **2016**, 6, 101216-101225	3.7	23
115	Ab Initio Thermodynamic and Thermophysical Properties of Sodium Metasilicate, NaSiO, and Their Electron-Density and Electron-Pair-Density Counterparts. *Journal of Physical Chemistry A*, **2016**, 120, 8881-8895	2.8	14
114	Source Function applied to experimental densities reveals subtle electron-delocalization effects and appraises their transferability properties in crystals. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2016**, 72, 180-93	1.8	20
113	Playing with isomerism and N substitution in pentalenedione derivatives for organic electrode batteries: how high are the stakes?. *Physical Chemistry Chemical Physics*, **2016**, 18, 2442-8	3.6	17
112	Heterointerface Electronic States and Charge Transport of Crystalline N,N′-1H,1H′-Perfluorobutil Dicyanoperylene Diimide in Field-Effect Transistor Configuration. *Journal of Physical Chemistry C*, **2016**, 120, 12083-12091	3.8	1
111	Exploring Chemistry Through the Source Function for the Electron and the Electron Spin Densities. *Challenges and Advances in Computational Chemistry and Physics*, **2016**, 101-129	0.7	3

110	Intermolecular Recognition of the Antimalarial Drug Chloroquine: A Quantum Theory of Atoms in Molecules Density Functional Theory Investigation of the Hydrated Dihydrogen Phosphate Salt from the 103 K X-ray Structure. *Crystal Growth and Design*, **2016**, 16, 6043-6054	3.5	14
109	Insights on spin polarization through the spin density source function. *Chemical Science*, **2015**, 6, 3845-3852	9.4	18
108	Engineering of unsubstituted quinoid-like frameworks enabling 2 V vs. Li(+)/Li redox voltage tunability and related derivatives. *Physical Chemistry Chemical Physics*, **2015**, 17, 8604-8	3.6	12
107	Energetics of non-covalent interactions from electron and energy density distributions. *Computational and Theoretical Chemistry*, **2015**, 1053, 53-59	2	45
106	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
105	Six questions on topology in theoretical chemistry. *Computational and Theoretical Chemistry*, **2015**, 1053, 2-16	2	81
104	Understanding the Reorientational Dynamics of Solid-State MBH4 (M = Li Cs). *Journal of Physical Chemistry C*, **2015**, 119, 12109-12118	3.8	6
103	Rationalizing the Lacking of Inversion Symmetry in a Noncentrosymmetric Polar Racemate: An Experimental and Theoretical Study. *Crystal Growth and Design*, **2014**, 14, 5822-5833	3.5	16
102	Single N C Bond Becomes Shorter than a Formally Double N?C Bond in a Thiazete-1,1-dioxide Crystal: An Experimental and Theoretical Study of Strong Crystal Field Effects. *Crystal Growth and Design*, **2014**, 14, 4418-4429	3.5	9
101	Relating Electrochemistry of New Organic Materials for Batteries and Fundamental Understanding through DFT Calculations. *Advances in Science and Technology*, **2014**, 93, 146-151	0.1	2
100	Electron Density Analysis **2013**, 187-226		17
99	The low/room-temperature forms of the lithiated salt of 3,6-dihydroxy-2,5-dimethoxy-p-benzoquinone: a combined experimental and dispersion-corrected density functional study. *CrystEngComm*, **2013**, 15, 2809	3.3	7
98	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
97	NCImilano: an electron-density-based code for the study of noncovalent interactions. *Journal of Applied Crystallography*, **2013**, 46, 1513-1517	3.8	44
96	Experimental and theoretical studies of tetramethoxy-p-benzoquinone: infrared spectra, structural and lithium insertion properties. *RSC Advances*, **2013**, 3, 19081	3.7	20
95	Challenging chemical concepts through charge density of molecules and crystals. *Physica Scripta*, **2013**, 87, 048102	2.6	31
94	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
93	Stability of xenon oxides at high pressures. *Nature Chemistry*, **2013**, 5, 61-5	17.6	101

92	Comparative study of X-ray charge-density data on CoSb3. *Acta Crystallographica Section A: Foundations and Advances*, **2013**, 69, 570-82		27
91	Strongly Correlated Intermetallics: (mathbf FeSb _mathbf{2}). *Springer Series in Materials Science*, **2013**, 71-93	0.9	
90	Non-covalent interaction via the reduced density gradient: Independent atom model vs experimental multipolar electron densities. *Computational and Theoretical Chemistry*, **2012**, 998, 148-163	2	98
89	Revealing non-covalent interactions in molecular crystals through their experimental electron densities. *Chemistry - A European Journal*, **2012**, 18, 15523-36	4.8	123
88	Energetics and bonding in aluminosilicate rings with alkali metal and alkaline-earth metal charge-compensating cations. *Journal of Physical Chemistry A*, **2012**, 116, 8584-98	2.8	9
87	Testing the concept of hypervalency: charge density analysis of K2SO4. *Inorganic Chemistry*, **2012**, 51, 8607-16	5.1	87
86	Revealing electron delocalization through the source function. *Journal of Physical Chemistry A*, **2011**, 115, 12864-78	2.8	48
85	A Guided Tour Through Modern Charge Density Analysis **2011**, 1-78		2
84	Challenging Problems in Charge Density Determination: Polar Bonds and Influence of the Environment. *Structure and Bonding*, **2011**, 47-97	0.9	14
83	The high-pressure phase of boron, □B28: Disputes and conclusions of 5 years after discovery. *Journal of Superhard Materials*, **2011**, 33, 363-379	0.9	32
82	The Source Function Descriptor as a Tool to Extract Chemical Information from Theoretical and Experimental Electron Densities. *Structure and Bonding*, **2011**, 193-285	0.9	43
81	13. Evolutionary Crystal Structure Prediction as a Method for the Discovery of Minerals and Materials **2010**, 271-298		4
80	Relativistic Effects on Metal-Metal Bonding: Comparison of the Performance of ECP and Scalar DKH Description on the Picture of Metal-Metal Bonding in Re2Cl8(2.). *Journal of Chemical Theory and Computation*, **2010**, 6, 3113-21	6.4	24
79	Evolutionary Crystal Structure Prediction as a Method for the Discovery of Minerals and Materials. *Reviews in Mineralogy and Geochemistry*, **2010**, 71, 271-298	7.1	143
78	Evolutionary Crystal Structure Prediction and Novel High-Pressure Phases. *NATO Science for Peace and Security Series B: Physics and Biophysics*, **2010**, 293-323	0.2	
77	Modeling environmental effects on charge density distributions in polar organometallics: validation of embedded cluster models for the methyl lithium crystal. *Journal of Computational Chemistry*, **2010**, 31, 2568-76	3.5	11
76	Vibrational properties of hexagonal Ge(2)Sb(2)Te(5) from first principles. *Journal of Physics Condensed Matter*, **2009**, 21, 245401	1.8	47
75	Ionic high-pressure form of elemental boron. *Nature*, **2009**, 457, 863-7	50.4	680

74	Ionic high-pressure form of elemental boron. *Nature*, **2009**, 460, 292	50.4	29
73	Using the Source Function descriptor to dampen the multipole model bias in charge density studies from X-ray structure factors refinements. *Chemical Physics Letters*, **2009**, 476, 308-316	2.5	23
72	Nature of the bonding in metal-silane sigma-complexes. *Inorganic Chemistry*, **2009**, 48, 1588-98	5.1	61
71	Do the structural changes defined by the electron density topology necessarily affect the picture of the bonding?. *Inorganic Chemistry*, **2009**, 48, 11024-31	5.1	45
70	Calcium filled skutterudites CaxCo4Sb12: effect of the computational approach on theab-initiomodeled electronic transport properties. *Journal of Physics: Conference Series*, **2008**, 117, 012010	0.3	1
69	Source function description of metal-metal bonding in d-block organometallic compounds. *Faraday Discussions*, **2007**, 135, 55-78; discussion 125-49, 503-6	3.6	118
68	Bond paths as privileged exchange channels. *Chemistry - A European Journal*, **2007**, 13, 9362-71	4.8	260
67	Chemical insight into electron density and wave functions: software developments and applications to crystals, molecular complexes and materials science. *Theoretical Chemistry Accounts*, **2007**, 117, 847-884	1.9	45
66	Chemical bonding in crystals: new directions. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2005**, 220,	1	447
65	Nanostructured Co1−xNix(Sb1−yTey)3 skutterudites: Theoretical modeling, synthesis and thermoelectric properties. *Journal of Applied Physics*, **2005**, 97, 044317	2.5	68
64	Beyond ?2Ð: chemical bond analysis using the local form of the source function. *Acta Crystallographica Section A: Foundations and Advances*, **2005**, 61, c47-c48		5
63	A Chemical Approacht o the First-Principles Modeling of Novel Thermoelectric Materials **2005**, 7-1-7-13		1
62	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
61	The local form of the source function as a fingerprint of strong and weak intra- and intermolecular interactions. *Acta Crystallographica Section A: Foundations and Advances*, **2004**, 60, 438-49		62
60	The Impact of Nanostructuring on the Thermal Conductivity of Thermoelectric CoSb3. *Advanced Functional Materials*, **2004**, 14, 1189-1196	15.6	239
59	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
58	Accuracy of topological analysis of gridded electron densities. *Journal of Physics and Chemistry of Solids*, **2004**, 65, 1951-1955	3.9	9
57	The impact of the actual geometrical structure of a thermoelectric material on its electronic transport properties: the case of doped skutterudite systems. *Journal of Chemical Physics*, **2004**, 121, 8983-9	3.9	50

56	Chemical information from the source function. *Journal of Computational Chemistry*, **2003**, 24, 422-36	3.5	147
55	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
54	The electron density in flavones I. Baicalein. *New Journal of Chemistry*, **2003**, 27, 1392-1398	3.6	20
53	Nanostructured Co1−xNixSb3 skutterudites: Synthesis, thermoelectric properties, and theoretical modeling. *Journal of Applied Physics*, **2003**, 93, 438-447	2.5	82
52	Fundamental Properties and Nature of CH···O Interactions in Crystals on the Basis of Experimental and Theoretical Charge Densities. The Case of 3,4-Bis(dimethylamino)-3-cyclobutene-1,2-dione (DMACB) Crystal. *Journal of Physical Chemistry A*, **2002**, 106, 2707-2720	2.8	107
51	Direct-space analysis of the Si–Si bonding pattern in the π-bonded chain reconstructed Si(111)(2 × 1) surface. *Theoretical Chemistry Accounts*, **2001**, 105, 309-322	1.9	8
50	The unexpected and large enhancement of the dipole moment in the 3,4-bis(dimethylamino)-3-cyclobutene-1,2-dione (DMACB) molecule upon crystallization: a new role of the intermolecular CH...O interactions. *Journal of the American Chemical Society*, **2001**, 123, 12248-54	16.4	51
49	Evaluation of net atomic charges and atomic and molecular electrostatic moments through topological analysis of the experimental charge density. *Acta Crystallographica Section A: Foundations and Advances*, **2000**, 56 (Pt 3), 252-8		132
48	On the origin of topological differences between experimental and theoretical crystal charge densities. *Acta Crystallographica Section A: Foundations and Advances*, **2000**, 56 (Pt 4), 332-9		118
47	Geometrical reconstructions and electronic relaxations of silicon surfaces. I. An electron density topological study of H-covered and clean Si(111)(1×1) surfaces. *Journal of Chemical Physics*, **2000**, 112, 887-899	3.9	15
46	Direct Space Representation of the Metallic Bond. *Journal of Physical Chemistry A*, **2000**, 104, 947-953	2.8	166
45	Shannon information entropies of molecules and functional groups in the self-consistent reaction field. *Journal of Chemical Physics*, **2000**, 112, 7572-7580	3.9	16
44	Steric and Electronic Effects in Methyl-Substituted 2,2′-Bipyrroles and Poly(2,2′-Bipyrrole)s: Part II. Theoretical Investigation on Monomers. *Chemistry of Materials*, **2000**, 12, 1490-1499	9.6	29
43	Steric and Electronic Effects in Methyl-Substituted 2,2′-Bipyrroles and Poly(2,2′-Bipyrrole)s: Part I. Synthesis and Characterization of Monomers and Polymers. *Chemistry of Materials*, **2000**, 12, 1480-1489	9.6	42
42	Evolution of energetics and bonding of compact self-interstitial clusters in Si. *Europhysics Letters*, **2000**, 50, 608-614	1.6	44
41	Interaction energy and density in the water dimer. A quantum theory of atoms in molecules: insight on the effect of basis set superposition error removal **2000**, 93-114		
40	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
39	A Green's function for the density. *Chemical Physics Letters*, **1998**, 287, 233-238	2.5	201

38	Rate enhancement of 1,3-dipolar cycloaddition of N-methylindole: the singular role of Grignard reagents **1998**, 11, 455-466		4
37	Molecular similarity based on information entropies and distances. *Journal of Chemical Physics*, **1998**, 108, 5469-5475	3.9	67
36	Formation and annihilation of a bond defect in silicon: An ab initio quantum-mechanical characterization. *Physical Review B*, **1998**, 57, 170-177	3.3	72
35	A theoretical investigation on the chemical bonding of interstitial and vacancy defects in silicon during their migration. *Nuclear Instruments & Methods in Physics Research B*, **1997**, 127-128, 235-238	1.2	2
34	TOPOND: a program for the application of the quantum theory of atoms in molecules to periodic systems. *Acta Crystallographica Section A: Foundations and Advances*, **1996**, 52, C555-C556		8
33	Theoretical and experimental (113 K) electron-density study of lithium bis(tetramethylammonium) hexanitrocobaltate(III). *Acta Crystallographica Section B: Structural Science*, **1996**, 52, 471-478		39
32	Dipole moment of the water molecule in the condensed phase: a periodic Hartree-Fock estimate. *Chemical Physics Letters*, **1995**, 247, 135-141	2.5	48
31	The electric field gradient at the N nuclei and the topology of the charge distribution in the protonation of urea. *Journal of Chemical Physics*, **1994**, 101, 9800-9806	3.9	6
30	Crystal field effects on the topological properties of the electron density in molecular crystals: The case of urea. *Journal of Chemical Physics*, **1994**, 101, 10686-10696	3.9	577
29	Are Bader electron populations atomic size dependent?. *The Journal of Physical Chemistry*, **1993**, 97, 11677-11680		87
28	Ab initio predictions of optically allowed transitions in Na20. Nature of excitations and influence of geometry. *Chemical Physics Letters*, **1993**, 213, 522-526	2.5	16
27	Nitranions and their precursors: charge density rearrangements and nitrogen-15 NMR chemical shift changes. *Journal of the American Chemical Society*, **1992**, 114, 8634-8644	16.4	34
26	Experimental vs. theoretical topological properties of charge density distributions. An application to the l-alanine molecule studied by X-ray diffraction at 23 K. *Computational and Theoretical Chemistry*, **1992**, 255, 409-433		56
25	Total electronic charge density of L-alanine from X-ray diffraction at 23 K. *Chemical Physics Letters*, **1991**, 186, 47-52	2.5	55
24	Search for cold fusion induced by electrolysis in palladium **1990**, 103, 1617-1638		4
23	On the choice of the perturbed state for pmo prediction of selectivities in cycloaddition reactions. *Computational and Theoretical Chemistry*, **1990**, 208, 235-251		3
22	A random phase approximation study of the absorption spectrum of Na8. *Chemical Physics Letters*, **1990**, 175, 645-654	2.5	16
21	Effect of electron correlation on the topological properties of molecular charge distributions. *Journal of Chemical Physics*, **1988**, 88, 3792-3804	3.9	87

20	Substituent effect on the planarization energy and the relative stability of Winstein and MÖbius structures of the homotropylium cation. *Computational and Theoretical Chemistry*, **1988**, 167, 275-300		5
19	Thermal rearrangements of the homotropylium cation: An MO investigation of some relevant stationary points on the potential energy surface. *Computational and Theoretical Chemistry*, **1988**, 166, 431-438		1
18	Properties of atoms in molecules: Dipole moments and transferability of properties. *Journal of Chemical Physics*, **1987**, 87, 1142-1152	3.9	184
17	Charge density topological study of bonding in lithium clusters. *Theoretica Chimica Acta*, **1987**, 72, 433-458		145
16	On the presence of non-nuclear attractors in the charge distributions of Li and Na clusters. *Chemical Physics Letters*, **1987**, 141, 380-385	2.5	154
15	Momoaromaticity versus mÖbius aromaticity. *Journal De Chimie Physique Et De Physico-Chimie Biologique*, **1987**, 84, 783-789		5
14	Cyclopropane ring closure in 11,11-disubstituted 1,6-methano [10] annulenes. *Computational and Theoretical Chemistry*, **1986**, 138, 39-50		17
13	Operational comparison of various thermodynamic treatments of organic substance adsorption at the electrode/solution interface. *Journal of Electroanalytical Chemistry and Interfacial Electrochemistry*, **1985**, 196, 179-197		13
12	Charge density topological approach to the dinorcaradiene .dblharw. [10]annulene equilibrium in some 11,11-disubstituted 1,6-methano[10]annulenes. *Journal of the American Chemical Society*, **1985**, 107, 878-887	16.4	38
11	The ring closure reaction in 1,6-methano-[10]annulene. *International Journal of Quantum Chemistry*, **1984**, 26, 433-438	2.1	3
10	A theoretical investigation on the role of solvent in solvolytic reactions. *Theoretica Chimica Acta*, **1983**, 63, 245-253		4
9	Generalized self-consistent valence bond method for ground and excited potential energy surfaces. *Molecular Physics*, **1980**, 41, 1259-1279	1.7	13
8	Pseudopotential calculations on hydrogen bonded systems : H2O, CH3OH and HCOOH dimers. *Molecular Physics*, **1979**, 38, 1865-1874	1.7	6
7	Solid State Applications of QTAIM and the Source Function Molecular Crystals, Surfaces, HostGuest Systems and Molecular Complexes163-206		2
6	Thermoelectric properties of nano-grained CoSb/sub 3/ skutterudites doped with Ni and Te		2
5	Standardisation in thermoelectric transport properties measurements - the Cardiff NEDO laboratories and DLR Cologne program		1
4	Thermoelectric performance of large single crystal clathrate Ba/sub 8/Ga/sub 16/Ge/sub 30/		2
3	Theoretical modeling of Te doped CoSb/sub 3/		1

2	Halide Perovskites: Advanced Photovoltaic Materials Empowered by a Unique Bonding Mechanism. *Advanced Functional Materials*,2110166	15.6	11
1	How to Identify Lone Pairs, Van der Waals Gaps, and Metavalent Bonding Using Charge and Pair Density Methods: From Elemental Chalcogens to Lead Chalcogenides and Phase-Change Materials. *Physica Status Solidi - Rapid Research Letters*,2000534	2.5	6