Mark A Spackman

List of Publications by Citations

134 papers	18,109 citations	45 h-index	134 g-index
139 ext. papers	21,116 ext. citations	4.3 avg, IF	7.25 L-index

#	Paper	IF	Citations
134	Hirshfeld surface analysis. *CrystEngComm*, **2009**, 11, 19-32	3.3	3999
133	Fingerprinting intermolecular interactions in molecular crystals. *CrystEngComm*, **2002**, 4, 378-392	3.3	2380
132	Towards quantitative analysis of intermolecular interactions with Hirshfeld surfaces. *Chemical Communications*, **2007**, 3814-6	5.8	2014
131	Novel tools for visualizing and exploring intermolecular interactions in molecular crystals. *Acta Crystallographica Section B: Structural Science*, **2004**, 60, 627-68		1741
130	A novel definition of a molecule in a crystal. *Chemical Physics Letters*, **1997**, 267, 215-220	2.5	787
129	Hirshfeld Surfaces: A New Tool for Visualising and Exploring Molecular Crystals. *Chemistry - A European Journal*, **1998**, 4, 2136-2141	4.8	556
128	model energies and energy frameworks: extension to metal coordination compounds, organic salts, solvates and open-shell systems. *IUCrJ*, **2017**, 4, 575-587	4.7	492
127	Comparing entire crystal structures: structural genetic fingerprinting. *CrystEngComm*, **2007**, 9, 648	3.3	378
126	: a program for Hirshfeld surface analysis, visualization and quantitative analysis of molecular crystals. *Journal of Applied Crystallography*, **2021**, 54, 1006-1011	3.8	344
125	Energy frameworks: insights into interaction anisotropy and the mechanical properties of molecular crystals. *Chemical Communications*, **2015**, 51, 3735-8	5.8	339
124	Visualisation and characterisation of voids in crystalline materials. *CrystEngComm*, **2011**, 13, 1804-1813	3.3	271
123	Accurate and Efficient Model Energies for Exploring Intermolecular Interactions in Molecular Crystals. *Journal of Physical Chemistry Letters*, **2014**, 5, 4249-55	6.4	258
122	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
121	Comparison of Polymorphic Molecular Crystal Structures through Hirshfeld Surface Analysis. *Crystal Growth and Design*, **2007**, 7, 755-769	3.5	235
120	Accurate prediction of static dipole polarizabilities with moderately sized basis sets. *The Journal of Physical Chemistry*, **1989**, 93, 7594-7603		219
119	A simple quantitative model of hydrogen bonding. *Journal of Chemical Physics*, **1986**, 85, 6587-6601	3.9	190
118	Atom□tom potentials via electron gas theory. *Journal of Chemical Physics*, **1986**, 85, 6579-6586	3.9	156

117	Solvent inclusion in the structural voids of form II carbamazepine: single-crystal X-ray diffraction, NMR spectroscopy and Hirshfeld surface analysis. *CrystEngComm*, **2007**, 9, 728	3.3	147
116	Potential derived charges using a geodesic point selection scheme **1996**, 17, 1-18		110
115	Accurate Lattice Energies for Molecular Crystals from Experimental Crystal Structures. *Journal of Chemical Theory and Computation*, **2018**, 14, 1614-1623	6.4	101
114	Molecules in crystals. *Physica Scripta*, **2013**, 87, 048103	2.6	101
113	Introduction and validation of an invariom database for amino-acid, peptide and protein molecules. *Acta Crystallographica Section D: Biological Crystallography*, **2006**, 62, 1325-35		87
112	Estimated H-atom anisotropic displacement parameters: a comparison between different methods and with neutron diffraction results. *Acta Crystallographica Section A: Foundations and Advances*, **2008**, 64, 465-75		85
111	Direct Evidence of Cation Disorder in Thermoelectric Lead Chalcogenides PbTe and PbS. *Advanced Functional Materials*, **2013**, 23, 5477-5483	15.6	83
110	Electrostatic potentials mapped on Hirshfeld surfaces provide direct insight into intermolecular interactions in crystals. *CrystEngComm*, **2008**,	3.3	83
109	Hydrogen bond energetics from topological analysis of experimental electron densities: Recognising the importance of the promolecule. *Chemical Physics Letters*, **1999**, 301, 425-429	2.5	83
108	How Reliable Are Intermolecular Interaction Energies Estimated from Topological Analysis of Experimental Electron Densities?. *Crystal Growth and Design*, **2015**, 15, 5624-5628	3.5	81
107	The Elusive Structural Origin of Plastic Bending in Dimethyl Sulfone Crystals with Quasi-isotropic Crystal Packing. *Angewandte Chemie - International Edition*, **2017**, 56, 8468-8472	16.4	80
106	Intermolecular interactions in molecular crystals: what's in a name?. *Faraday Discussions*, **2017**, 203, 93-112	3.6	76
105	Vibrational averaging of electrical properties. *Molecular Physics*, **1995**, 84, 1239-1255	1.7	75
104	Dipole moment enhancement in molecular crystals from X-ray diffraction data. *ChemPhysChem*, **2007**, 8, 2051-63	3.2	63
103	Reassessment of large dipole moment enhancements in crystals: a detailed experimental and theoretical charge density analysis of 2-methyl-4-nitroaniline. *Journal of Physical Chemistry A*, **2006**, 110, 8763-76	2.8	61
102	Anisotropic displacement parameters for H atoms using an ONIOM approach. *Acta Crystallographica Section B: Structural Science*, **2006**, 62, 875-88		59
101	Anisotropic molecular polarizabilities, dipole moments, and quadrupole moments of (CH2)2X, (CH3)2X, and C4H4X (X = O, S, Se). Comparison of experimental results and ab initio calculations. *The Journal of Physical Chemistry*, **1992**, 96, 7301-7307		54
100	Electron distribution and molecular motion in crystalline benzene: an accurate experimental study combining CCD X-ray data on C6H6 with multitemperature neutron-diffraction results on C6D6. *Chemistry - A European Journal*, **2002**, 8, 3512-21	4.8	53

99	Influence of intermolecular interactions on multipole-refined electron densities. *Acta Crystallographica Section A: Foundations and Advances*, **1999**, 55, 30-47		53
98	Time-dependent Hartree–Fock second-order molecular properties with a moderately sized basis set. I. The frequency dependence of the dipole polarizability. *Journal of Chemical Physics*, **1991**, 94, 1288-1294	3.9	53
97	Basis set choice and basis set superposition error (BSSE) in periodic Hartree–Fock calculations on molecular crystals. *Physical Chemistry Chemical Physics*, **2001**, 3, 1518-1523	3.6	52
96	An ab initio study of vibrational corrections to the electrical properties of the second-row hydrides. *Molecular Physics*, **1997**, 90, 251-264	1.7	51
95	Molecular surfaces from the promolecule: A comparison with Hartree–Fock ab initio electron density surfaces. *Journal of Computational Chemistry*, **2000**, 21, 933-942	3.5	51
94	A simple quantitative model of hydrogen bonding: application to more complex systems. *The Journal of Physical Chemistry*, **1987**, 91, 3179-3186		51
93	Invarioms for improved absolute structure determination of light-atom crystal structures. *Acta Crystallographica Section A: Foundations and Advances*, **2006**, 62, 217-23		48
92	Accurate prediction of static dipole polarizabilities with moderately sized basis sets. *Molecular Physics*, **1994**, 82, 193-209	1.7	48
91	Hirshfeld atom refinement for modelling strong hydrogen bonds. *Acta Crystallographica Section A: Foundations and Advances*, **2014**, 70, 483-98	1.7	47
90	Visualizing lithium-ion migration pathways in battery materials. *Chemistry - A European Journal*, **2013**, 19, 15535-44	4.8	45
89	Molecular dynamics simulations of structure and dynamics of organic molecular crystals. *Physical Chemistry Chemical Physics*, **2010**, 12, 14916-29	3.6	43
88	The use of the promolecular charge density to approximate the penetration contribution to intermolecular electrostatic energies. *Chemical Physics Letters*, **2006**, 418, 158-162	2.5	43
87	Polymorphism in 3-methyl-4-methoxy-4?-nitrostilbene (MMONS), a highly active NLO material. *CrystEngComm*, **2008**, 10, 197-206	3.3	42
86	Effective molecular polarizabilities and crystal refractive indices estimated from x-ray diffraction data. *Journal of Chemical Physics*, **2006**, 125, 174505	3.9	42
85	Synthesis, crystal structure, atomic Hirshfeld surfaces, and physical properties of hexagonal CeMnNi4. *Inorganic Chemistry*, **2010**, 49, 9343-9	5.1	40
84	Energy frameworks and a topological analysis of the supramolecular features in in situ cryocrystallized liquids: tuning the weak interaction landscape via fluorination. *Physical Chemistry Chemical Physics*, **2016**, 18, 31811-31820	3.6	39
83	Charge density analysis of two polymorphs of antimony(III) oxide. *Dalton Transactions*, **2004**, 23-9	4.3	39
82	Crystal packing in the 2-R,4-oxo-[1,3-a/b]-naphthodioxanes – Hirshfeld surface analysis and melting point correlation. *CrystEngComm*, **2012**, 14, 1083-1093	3.3	38

81	Refractive indices for molecular crystals from the response of X-ray constrained Hartree-Fock wavefunctions. *Physical Chemistry Chemical Physics*, **2009**, 11, 7209-18	3.6	37
80	The use of dipole lattice sums to estimate electric fields and dipole moment enhancement in molecular crystals. *Chemical Physics Letters*, **2007**, 443, 87-91	2.5	37
79	Can the interaction density be measured? The example of the non-standard amino acid sarcosine. *Acta Crystallographica Section A: Foundations and Advances*, **2007**, 63, 426-36		37
78	Redetermination, invariom-model and multipole refinement of L-ornithine hydrochloride. *Acta Crystallographica Section B: Structural Science*, **2007**, 63, 505-9		36
77	Time-dependent Hartree–Fock second-order molecular properties with a moderately sized basis set. II. Dispersion coefficients. *Journal of Chemical Physics*, **1991**, 94, 1295-1305	3.9	36
76	'Quasi-isostructural polymorphism' in molecular crystals: inputs from interaction hierarchy and energy frameworks. *Chemical Communications*, **2016**, 52, 2141-4	5.8	35
75	Accurate ab initio study of acetylene Vibrational and rotational corrections to electrical properties. *Molecular Physics*, **1996**, 88, 1109-1136	1.7	35
74	Magnetically recoverable FeO@Au-coated nanoscale catalysts for the A-coupling reaction. *Dalton Transactions*, **2017**, 46, 5133-5137	4.3	34
73	Bond length and local energy density property connections for non-transition-metal oxide-bonded interactions. *Journal of Physical Chemistry A*, **2006**, 110, 12259-66	2.8	31
72	An Exploration of Theoretical and Experimental Electron Density Distributions and SiO Bonded Interactions for the Silica Polymorph Coesite. *Journal of Physical Chemistry B*, **2003**, 107, 12996-13006	3.4	31
71	Chapter 5. Charge densities from X-ray diffraction data. *Annual Reports on the Progress of Chemistry Section C*, **1998**, 94, 177		30
70	Electrostatic potential in dehydrated zeolite NaA from low-resolution x-ray diffraction data. *The Journal of Physical Chemistry*, **1988**, 92, 794-796		29
69	The Elusive Structural Origin of Plastic Bending in Dimethyl Sulfone Crystals with Quasi-isotropic Crystal Packing. *Angewandte Chemie*, **2017**, 129, 8588-8592	3.6	28
68	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
67	Theoretical electron density distributions for Fe- and Cu-sulfide earth materials: a connection between bond length, bond critical point properties, local energy densities, and bonded interactions. *Journal of Physical Chemistry B*, **2007**, 111, 1923-31	3.4	26
66	The Polymorphs of ROY: A Computational Study of Lattice Energies and Conformational Energy Differences. *Australian Journal of Chemistry*, **2018**, 71, 279	1.2	25
65	Supramolecular polymorphism of the 1:1 molecular salt (adamantane-1-carboxylate-3,5,7-tricarboxylic acid)·(hexamethylenetetraminium). A "failed" crystal engineering attempt. *Chemical Communications*, **2012**, 48, 1883-5	5.8	25
64	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

63	Controlling the confinement and alignment of fullerene C(70) in para-substituted calix[5]arenes. *Chemistry - A European Journal*, **2007**, 13, 3907-12	4.8	25
62	Supramolecular Recognition and Energy Frameworks in Host□Guest Complexes of 18-Crown-6 and Sulfonamides. *Crystal Growth and Design*, **2015**, 15, 5892-5900	3.5	23
61	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
60	Visualising intermolecular interactions in crystals: naphthalene vs. terephthalic acid. *Chemical Communications*, **1998**, 2071-2072	5.8	23
59	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
58	Analysis of the compression of molecular crystal structures using Hirshfeld surfaces. *CrystEngComm* , **2008**,	3.3	21
57	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
56	Supramolecular interactions between hexabromoethane and cyclopentadienyl ruthenium bromides: Halogen bonding or electrostatic organisation?. *CrystEngComm*, **2012**, 14, 804-811	3.3	19
55	Mechanism of concerted hydrogen bond reorientation in clathrates of Dianin's compound and hydroquinone. *Journal of the American Chemical Society*, **2011**, 133, 18880-8	16.4	18
54	Variable Intercalation of Calcium Ions in Bilayers of Partially Deprotonated p-Phosphonic Acid Calix[4]arene. *Crystal Growth and Design*, **2009**, 9, 3759-3764	3.5	18
53	Intermolecular Interaction Energies in Hydroquinone Clathrates at High Pressure. *Crystal Growth and Design*, **2017**, 17, 3834-3846	3.5	17
52	An ab initio study of vibrational corrections to the electrical properties of ethylene. *Molecular Physics*, **2000**, 98, 855-865	1.7	17
51	Ectrostatic Potentials in Crystals **1981**, 407-425		17
50	Molecular Imprisonment: Host Response to Guest Location, Orientation, and Dynamics in Clathrates of Dianin□ Compound. *Crystal Growth and Design*, **2014**, 14, 1296-1306	3.5	16
49	Simulations of guest transport in clathrates of Dianin's compound and hydroquinone. *Chemistry - A European Journal*, **2013**, 19, 2676-84	4.8	16
48	Revisiting a Historical Concept by Using Quantum Crystallography: Are Phosphate, Sulfate and Perchlorate Anions Hypervalent?. *Chemistry - A European Journal*, **2019**, 25, 6523-6532	4.8	15
47	Crystal structure and chemical bonding of the intermetallic Zintl phase Yb11AlSb9. *Dalton Transactions*, **2012**, 41, 10347-53	4.3	15
46	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

45	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
44	Variable temperature Hirshfeld surface analysis of interdigitated calix[6]arene bearing O-alkyl C18 linear chains. *CrystEngComm*, **2007**, 9, 566	3.3	14
43	The determination of electric field gradients from X-ray diffraction data. *Molecular Physics*, **1994**, 83, 551-566	1.7	14
42	Bridging Crystal Engineering and Drug Discovery by Utilizing Intermolecular Interactions and Molecular Shapes in Crystals. *Angewandte Chemie - International Edition*, **2019**, 58, 16780-16784	16.4	13
41	Si-O bonded interactions in silicate crystals and molecules: a comparison. *Journal of Physical Chemistry A*, **2006**, 110, 12678-83	2.8	13
40	Ab initio SCF and MP2 calculations of the frequency dependence of the polarizability of cyclohexane. *Chemical Physics Letters*, **1989**, 161, 285-290	2.5	13
39	Dipole and quadrupole moments of molecules in crystals: a novel approach based on integration over Hirshfeld surfaces. *Journal of Chemical Physics*, **2006**, 124, 74106	3.9	12
38	Global Analysis of the Mechanical Properties of Organic Crystals. *Angewandte Chemie - International Edition*, **2021**,	16.4	12
37	Quantifying Host□Guest Interaction Energies in Clathrates of Dianin□s Compound. *Crystal Growth and Design*, **2016**, 16, 6858-6866	3.5	11
36	Pauling bond strength, bond length and electron density distribution. *Physics and Chemistry of Minerals*, **2014**, 41, 17-25	1.6	11
35	Electrostatic complementarity in pseudoreceptor modeling based on drug molecule crystal structures: the case of loxistatin acid (E64c). *New Journal of Chemistry*, **2015**, 39, 1628-1633	3.6	10
34	Revised electrostatics from invariom refinement of the 18-residue peptaibol antibiotic trichotoxin A50E. *CrystEngComm*, **2010**, 12, 2419	3.3	10
33	Comment on On the calculation of the electrostatic potential, electric field and electric field gradient from the aspherical pseudoatom model by Volkov, King, Coppens & Farrugia (2006). *Acta Crystallographica Section A: Foundations and Advances*, **2007**, 63, 198-200; author reply 201-3		10
32	An ab initio study of vibrational corrections to the electrical properties of ethane. *Molecular Physics* , **2000**, 98, 867-874	1.7	10
31	An ab initio study of vibrational corrections to the electrical properties of the fluoromethanes: CH3F, CH2F2, CHF3 and CF4. *Molecular Physics*, **2000**, 98, 633-642	1.7	10
30	Properties of atoms under pressure: bonded interactions of the atoms in three perovskites. *Journal of Chemical Physics*, **2012**, 137, 164313	3.9	9
29	Computational study of methyl group dynamics in the hydroquinone clathrate of acetonitrile. *Physical Chemistry Chemical Physics*, **2012**, 14, 1570-2	3.6	9
28	Temperature-dependent crystal structure of the isopropanol clathrate of Dianin's compound. *Chemical Communications*, **2011**, 47, 2029-31	5.8	9

27	Ab initio cluster calculations of the electron density and electric field gradient in corundum. *The Journal of Physical Chemistry*, **1992**, 96, 9200-9204		9
26	Host perturbation in a 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
25	Proton switching of polarity in metalloamphiphile crystals. *CrystEngComm*, **2009**, 11, 249-253	3.3	8
24	Combined structure-factor phase measurement and theoretical calculations for mapping of chemical bonds in GaN. *Acta Crystallographica Section A: Foundations and Advances*, **2010**, 66, 446-50		7
23	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
22	Towards the use of experimental electron densities to estimate reliable lattice energies. *CrystEngComm*, **2018**, 20, 5340-5347	3.3	6
21	Invariom-model refinement of L-valinol. *Acta Crystallographica Section C: Crystal Structure Communications*, **2006**, 62, o633-5		6
20	Electric field-derived point charges to mimic the electrostatics in molecular crystals. *Journal of Computational Chemistry*, **2006**, 27, 1063-70	3.5	5
19	Global Analysis of the Mechanical Properties of Organic Crystals. *Angewandte Chemie*,	3.6	5
18	Approaching an experimental electron density model of the biologically active trans-epoxysuccinyl amide group Substituent effects vs. crystal packing. *Journal of Physical Organic Chemistry*, **2017**, 30, e3683	2.1	4
17	Tetraiodoallene, I2C=C=CI2 the missing link between I2C=CI2 and I2C=C=C=CI2 and the oxidation product, 2,2-diiodoacrylicacid, I2C=CH(CO2H). *Australian Journal of Chemistry*, **2018**, 71, 70	1.2	4
16	Phase measurement for accurate mapping of chemical bonds in acentric space groups. *Physical Review Letters*, **2005**, 95, 085502	7.4	4
15	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
14	Bridging Crystal Engineering and Drug Discovery by Utilizing Intermolecular Interactions and Molecular Shapes in Crystals. *Angewandte Chemie*, **2019**, 131, 16936-16940	3.6	3
13	Seemingly simple group 8 cyclopentadienyl dicarbonyl metal halides: From little things, interesting things grow. *CrystEngComm*, **2012**, 14, 812-818	3.3	3
12	Physical and crystallographic characterisation of the mGlu5 antagonist MTEP and its monohydrochloride. *Journal of Pharmaceutical Sciences*, **2010**, 99, 234-45	3.9	3
11	Accurate ab initio study of acetylene Vibrational and rotational corrections to electrical properties		3
10	Single-Crystal High-Pressure X-ray Diffraction Study of Host Structure Compression in Clathrates of Dianin Compound. *Crystal Growth and Design*, **2020**, 20, 4092-4099	3.5	2

9	Intermolecular interactions in crystals of small unsubstituted cyclic ethers and substituted epoxides. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2018**, 233, 641-648	1	2
8	Quantifying Mechanical Properties of Molecular Crystals: A Critical Overview of Experimental Elastic Tensors. *Angewandte Chemie - International Edition*, **2021**,	16.4	2
7	Geometries, interaction energies and complexation free energies of 18-crown-6 with neutral molecules. *CrystEngComm*, **2016**, 18, 8653-8663	3.3	1
6	Facile Synthesis of Pentamethylcyclopentadienyl Ruthenium Half-Sandwich Complexes by Naphthalene Displacement. *Australian Journal of Chemistry*, **2018**, 71, 289	1.2	1
5	Charge Densities and Crystal Engineering **2011**, 553-572		1
4	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
3	Robert Farrell Stewart (1936-2015). *Acta Crystallographica Section A: Foundations and Advances*, **2016**, 72, 507-9	1.7	
2	Contracted basis sets for electrical property calculations derived from Second-order M□ller□Plesset theory atomic natural orbitals. *Theoretical Chemistry Accounts*, **2000**, 104, 385-391	1.9	
1	Structure correlation and dynamics in crystals □a tribute to Hans-Beat B□rgi. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2022**, 78, 281-282	1.8	