Dylan Jayatilaka

List of Publications by Citations

133 papers	12,706 citations	43 h-index	112 g-index
155 ext. papers	15,166 ext. citations	3.3 avg, IF	6.94 L-index

#	Paper	IF	Citations
133	Hirshfeld surface analysis. *CrystEngComm*, **2009**, 11, 19-32	3.3	3999
132	Towards quantitative analysis of intermolecular interactions with Hirshfeld surfaces. *Chemical Communications*, **2007**, 3814-6	5.8	2014
131	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
130	Comparing entire crystal structures: structural genetic fingerprinting. *CrystEngComm*, **2007**, 9, 648	3.3	378
129	: a program for Hirshfeld surface analysis, visualization and quantitative analysis of molecular crystals. *Journal of Applied Crystallography*, **2021**, 54, 1006-1011	3.8	344
128	Energy frameworks: insights into interaction anisotropy and the mechanical properties of molecular crystals. *Chemical Communications*, **2015**, 51, 3735-8	5.8	339
127	Visualisation and characterisation of voids in crystalline materials. *CrystEngComm*, **2011**, 13, 1804-1813	3.3	271
126	Accurate and Efficient Model Energies for Exploring Intermolecular Interactions in Molecular Crystals. *Journal of Physical Chemistry Letters*, **2014**, 5, 4249-55	6.4	258
125	Ab initio calculation of anharmonic constants for a transition state, with application to semiclassical transition state tunneling probabilities. *Chemical Physics Letters*, **1990**, 172, 62-68	2.5	193
124	Open-shell coupled-cluster theory. *Journal of Chemical Physics*, **1993**, 98, 9734-9747	3.9	158
123	Hydrogen atoms can be located accurately and precisely by x-ray crystallography. *Science Advances*, **2016**, 2, e1600192	14.3	147
122	Hirshfeld atom refinement. *IUCrJ*, **2014**, 1, 361-79	4.7	140
121	Higher analytic derivatives. IV. Anharmonic effects in the benzene spectrum. *Journal of Chemical Physics*, **1992**, 97, 4233-4254	3.9	139
120	An open-shell restricted Hartree–Fock perturbation theory based on symmetric spin orbitals. *Chemical Physics Letters*, **1993**, 201, 1-10	2.5	136
119	Wavefunctions derived from experiment. I. Motivation and theory. *Acta Crystallographica Section A: Foundations and Advances*, **2001**, 57, 76-86		135
118	X-ray structure refinement using aspherical atomic density functions obtained from quantum-mechanical calculations. *Acta Crystallographica Section A: Foundations and Advances*, **2008**, 64, 383-93		124
117	Anharmonic corrections to vibrational transition intensities. *The Journal of Physical Chemistry*, **1990**, 94, 5608-5616		119

116	Wave Function for Beryllium from X-Ray Diffraction Data. *Physical Review Letters*, **1998**, 80, 798-801	7.4	112
115	Anharmonic vibrational properties of CH2F2 : A comparison of theory and experiment. *Journal of Chemical Physics*, **1991**, 95, 8323-8336	3.9	110
114	Accurate Lattice Energies for Molecular Crystals from Experimental Crystal Structures. *Journal of Chemical Theory and Computation*, **2018**, 14, 1614-1623	6.4	101
113	The prediction of spectroscopic properties from quartic correlated force fields: HCCF, HFCO, SiH+3. *Journal of Chemical Physics*, **1990**, 93, 4965-4981	3.9	94
112	The predominant role of coordination number in potassium channel selectivity. *Biophysical Journal*, **2007**, 93, 2635-43	2.9	93
111	Open-shell restricted Hartree□ock perturbation theory: Some considerations and comparisons. *Journal of Chemical Physics*, **1994**, 100, 7400-7409	3.9	89
110	The significance of ionic bonding in sulfur dioxide: bond orders from X-ray diffraction data. *Angewandte Chemie - International Edition*, **2012**, 51, 6776-9	16.4	83
109	Electrostatic potentials mapped on Hirshfeld surfaces provide direct insight into intermolecular interactions in crystals. *CrystEngComm*, **2008**,	3.3	83
108	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
107	Tonto: A Fortran Based Object-Oriented System for Quantum Chemistry and Crystallography. *Lecture Notes in Computer Science*, **2003**, 142-151	0.9	78
106	Quantum Crystallography: Current Developments and Future Perspectives. *Chemistry - A European Journal*, **2018**, 24, 10881-10905	4.8	77
105	Intermolecular interactions in molecular crystals: what's in a name?. *Faraday Discussions*, **2017**, 203, 93-112	3.6	76
104	A flexible approach to the calculation of resonance energy transfer efficiency between multiple donors and acceptors in complex geometries. *Biophysical Journal*, **2005**, 89, 3822-36	2.9	76
103	Spin contamination in single-determinant wavefunctions. *Chemical Physics Letters*, **1991**, 183, 423-431	2.5	76
102	Electron spin resonance g tensors from general Hartree□ock calculations. *Journal of Chemical Physics*, **1998**, 108, 7587-7594	3.9	72
101	Wavefunctions derived from experiment. II. A wavefunction for oxalic acid dihydrate. *Acta Crystallographica Section A: Foundations and Advances*, **2001**, 57, 87-100		70
100	Probing the accuracy and precision of Hirshfeld atom refinement with interfaced with. *IUCrJ*, **2018**, 5, 32-44	4.7	60
99	Higher analytic derivatives. II. The fourth derivative of self-consistent-field energy. *Journal of Chemical Physics*, **1991**, 95, 7409-7417	3.9	53

98	S···O chalcogen bonding in sulfa drugs: insights from multipole charge density and X-ray wavefunction of acetazolamide. *Physical Chemistry Chemical Physics*, **2015**, 17, 25411-20	3.6	52
97	Wave functions derived from experiment. V. Investigation of electron densities, electrostatic potentials, and electron localization functions for noncentrosymmetric crystals. *Journal of Computational Chemistry*, **2003**, 24, 470-83	3.5	49
96	Hirshfeld atom refinement for modelling strong hydrogen bonds. *Acta Crystallographica Section A: Foundations and Advances*, **2014**, 70, 483-98	1.7	47
95	Ab initio prediction of fundamental, overtone and combination band infrared intensities. *Chemical Physics Letters*, **1990**, 169, 127-137	2.5	47
94	Importance of Relativistic Effects and Electron Correlation in Structure Factors and Electron Density of Diphenyl Mercury and Triphenyl Bismuth. *Journal of Physical Chemistry A*, **2016**, 120, 6650-69	2.8	45
93	Determination of the orientational distribution and orientation factor for transfer between membrane-bound fluorophores using a confocal microscope. *Biophysical Journal*, **2006**, 91, 1032-45	2.9	44
92	Wavefunctions derived from experiment. IV. Investigation of the crystal environment of ammonia. *Acta Crystallographica Section A: Foundations and Advances*, **2002**, 58, 244-51		44
91	Higher analytic derivatives. I. A new implementation for the third derivative of the SCF energy. *International Journal of Quantum Chemistry*, **1991**, 40, 179-199	2.1	43
90	Effective molecular polarizabilities and crystal refractive indices estimated from x-ray diffraction data. *Journal of Chemical Physics*, **2006**, 125, 174505	3.9	42
89	The form of spin orbitals for open-shell restricted Hartree–Fock reference functions. *Chemical Physics Letters*, **1992**, 199, 211-219	2.5	41
88	Accurate crystal structures and chemical properties from NoSpherA2. *Chemical Science*, **2020**, 12, 1675-1692	9.4	41
87	Wavefunctions derived from experiment. III. Topological analysis of crystal fragments. *Acta Crystallographica Section A: Foundations and Advances*, **2002**, 58, 232-43		40
86	Some fundamental problems with zero flux partitioning of electron densities. *Theoretical Chemistry Accounts*, **2001**, 105, 213-218	1.9	40
85	X-ray constrained unrestricted Hartree-Fock and Douglas-Kroll-Hess wavefunctions. *Acta Crystallographica Section A: Foundations and Advances*, **2010**, 66, 78-92		39
84	Basis set convergence of CCSD(T) equilibrium geometries using a large and diverse set of molecular structures. *Journal of Chemical Physics*, **2016**, 145, 104101	3.9	38
83	Reversible hydrogen storage properties of defect-engineered C4N nanosheets under ambient conditions. *Carbon*, **2019**, 152, 344-353	10.4	37
82	Structural investigation of MscL gating using experimental data and coarse grained MD simulations. *PLoS Computational Biology*, **2012**, 8, e1002683	5	37
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	Electron localization functions obtained from X-ray constrained Hartree-Fock wavefunctions for molecular crystals of ammonia, urea and alloxan. *Acta Crystallographica Section A: Foundations and Advances*, **2004**, 60, 111-9		37
78	Simulation of structure, orientation, and energy transfer between AlexaFluor molecules attached to MscL. *Biophysical Journal*, **2008**, 95, 2711-21	2.9	35
77	Validation of X-ray Wavefunction Refinement. *ChemPhysChem*, **2017**, 18, 3334-3351	3.2	34
76	Crystal-field effects inL-homoserine: multipolesversusquantum chemistry. *Acta Crystallographica Section A: Foundations and Advances*, **2012**, 68, 435-442		31
75	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
74	Higher analytic derivatives. *Molecular Physics*, **1992**, 75, 271-291	1.7	29
73	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
72	Covalency and Ionicity Do Not Oppose Each Other-Relationship Between Si-O Bond Character and Basicity of Siloxanes. *Chemistry - A European Journal*, **2018**, 24, 15275-15286	4.8	28
71	The electron localizability indicator from X-ray diffraction data--a first application to a series of epoxide derivatives. *Chemistry - A European Journal*, **2010**, 16, 12818-21	4.8	27
70	A comparison of electron density from Hirshfeld-atom refinement, X-ray wavefunction refinement and multipole refinement on three urea derivatives. *CrystEngComm*, **2013**, 15, 2084	3.3	26
69	Modeling electron density distributions from X-ray diffraction to derive optical properties: constrained wavefunction versus multipole refinement. *Journal of Chemical Physics*, **2013**, 139, 064108	3.9	25
68	A definition for the covalent and ionic bond index in a molecule. *Theoretical Chemistry Accounts*, **2008**, 119, 275-290	1.9	25
67	A Variety of Bond Analysis Methods, One Answer? An Investigation of the Element-Oxygen Bond of Hydroxides H XOH. *Chemistry - A European Journal*, **2018**, 24, 6248-6261	4.8	24
66	A challenge for density functional theory: the XONO and XNO2 (X=F, Cl, and Br) molecules. *Theoretical Chemistry Accounts*, **1997**, 97, 185-194	1.9	23
65	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
64	Metal functionalized inorganic nano-sheets as promising materials for clean energy storage. *Applied Surface Science*, **2019**, 471, 887-892	6.7	23
63	Reactivity differences between α,β-unsaturated carbonyls and hydrazones investigated by experimental and theoretical electron density and electron localizability analyses. *Journal of Physical Chemistry A*, **2011**, 115, 12715-32	2.8	21

62	Fourier transforms of property densities with Gaussian functions. *Chemical Physics Letters*, **1994**, 230, 228-230	2.5	21
61	Die Bedeutung ionischer Bindungsanteile in Schwefeldioxid Bindungsordnungen aus Röntgenbeugungsdaten. *Angewandte Chemie*, **2012**, 124, 6880-6884	3.6	20
60	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
59	High Throughput Profiling of Molecular Shapes in Crystals. *Scientific Reports*, **2016**, 6, 22204	4.9	20
58	Testing the use of molecular dynamics to simulate fluorophore motions and FRET. *Physical Chemistry Chemical Physics*, **2011**, 13, 11045-54	3.6	18
57	Hydrogen atoms in bridging positions from quantum crystallographic refinements: influence of hydrogen atom displacement parameters on geometry and electron density. *CrystEngComm*, **2020**, 22, 4778-4789	3.3	17
56	Predicting the Position of the Hydrogen Atom in the Short Intramolecular Hydrogen Bond of the Hydrogen Maleate Anion from Geometric Correlations. *Crystal Growth and Design*, **2017**, 17, 3812-3825	3.5	16
55	Relativistic quantum crystallography of diphenyl- and dicyanomercury. Theoretical structure factors and Hirshfeld atom refinement. *Acta Crystallographica Section A: Foundations and Advances*, **2019**, 75, 705-717	1.7	16
54	Mapping the importance of four factors in creating monovalent ion selectivity in biological molecules. *Biophysical Journal*, **2011**, 100, 60-9	2.9	16
53	Comparison of semiempirical and ab initio QM decomposition analyses for the interaction energy between molecules. *Chemical Physics Letters*, **2002**, 352, 245-251	2.5	16
52	Bond orders for intermolecular interactions in crystals: charge transfer, ionicity and the effect on intramolecular bonds. *IUCrJ*, **2018**, 5, 635-646	4.7	16
51	Reliable Measurements of Dipole Moments from Single-Crystal Diffraction Data and Assessment of an In-Crystal Enhancement. *Structure and Bonding*, **2012**, 27-45	0.9	15
50	Post-Hartree-Fock methods for Hirshfeld atom refinement: are they necessary? Investigation of a strongly hydrogen-bonded molecular crystal. *Journal of Molecular Structure*, **2020**, 1209, 127934	3.4	14
49	ExiFRET: flexible tool for understanding FRET in complex geometries. *Journal of Biomedical Optics*, **2012**, 17, 011005	3.5	14
48	A problematic issue for atoms in molecules: Impact of (quasi-)degenerate states on Quantum Theory Atoms in Molecules and Hirshfeld-I properties. *Computational and Theoretical Chemistry*, **2015**, 1053, 106-111	2	13
47	The Advent of Quantum Crystallography: Form and Structure Factors from Quantum Mechanics for Advanced Structure Refinement and Wavefunction Fitting. *Structure and Bonding*, **2020**, 65-144	0.9	13
46	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
45	Picture change error correction of radon atom electron density. *Journal of Chemical Physics*, **2010**, 133, 174125	3.9	13

44	Si-O bonded interactions in silicate crystals and molecules: a comparison. *Journal of Physical Chemistry A*, **2006**, 110, 12678-83	2.8	13
43	An ab initio calculation of magnetic structure factors for Cs3CoCl5 including spin□orbit and finite magnetic field effects. *Journal of Chemical Physics*, **1995**, 103, 4562-4571	3.9	13
42	Picture change error in quasirelativistic electron/spin density, Laplacian and bond critical points. *Chemical Physics*, **2014**, 438, 37-47	2.3	12
41	Study of the picture change error at the 2nd order Douglas Kroll Hess level of theory. Electron and spin density and structure factors of the Bis[bis(methoxycarbimido) aminato] copper (II) complex. *Chemical Physics*, **2012**, 395, 44-53	2.3	12
40	On the accuracy and precision of X-ray and neutron diffraction results as a function of resolution and the electron density model. *IUCrJ*, **2020**, 7, 920-933	4.7	12
39	Are intramolecular dynamic electron correlation effects detectable in X-ray diffraction experiments on molecular crystals?. *Acta Crystallographica Section A: Foundations and Advances*, **2007**, 63, 135-45		11
38	Spin contamination analogy, Kramers pairs symmetry and spin density representations at the 2-component unrestricted Hartree□ock level of theory. *Computational and Theoretical Chemistry*, **2015**, 1065, 27-41	2	10
37	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
36	Solid-State Dilution of Dihydroxybenzophenones with 4,13-Diaza-18-crown-6 for Photocrystallographic Studies. *Crystal Growth and Design*, **2012**, 12, 2277-2287	3.5	10
35	Picture change error correction in the radial distributions of canonical orbital densities and total electron density of radon atom: the effect of the size of nucleus and the basis set limit. *Theoretical Chemistry Accounts*, **2011**, 129, 181-197	1.9	10
34	Revised electrostatics from invariom refinement of the 18-residue peptaibol antibiotic trichotoxin A50E. *CrystEngComm*, **2010**, 12, 2419	3.3	10
33	Analytic second derivatives with model potentials at SCF and MP2 levels. *Chemical Physics Letters*, **1989**, 163, 151-156	2.5	10
32	Cyclopropa-Fused Quinones. The Generation and Trapping of Bicyclo[4.1.0]hepta-1(6),3-diene-2,5-dione and 1H-Cyclopropa[b]naphthalene-2,7-dione. *Australian Journal of Chemistry*, **1997**, 50, 505	1.2	10
31	Linear MgCp* vs Bent CaCp*: London Dispersion, Ligand-Induced Charge Localizations, and Pseudo-Pregostic C-H□□Ca Interactions. *Inorganic Chemistry*, **2018**, 57, 4906-4920	5.1	9
30	Predicting the primary fragments in mass spectrometry using ab initio Roby□ould bond indices. *International Journal of Quantum Chemistry*, **2018**, 118, e25603	2.1	9
29	An entropic mechanism of generating selective ion binding in macromolecules. *PLoS Computational Biology*, **2013**, 9, e1002914	5	9
28	Can Experimental Electron-Density Studies be Used as a Tool to Predict Biologically Relevant Properties of Low-Molecular Weight Enzyme Ligands?. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2013**, 639, 1905-1921	1.3	9
27	A complement to □ome fundamental problems with zero flux partitioning of electron densities□ *Theoretical Chemistry Accounts*, **2002**, 107, 383-384	1.9	9

26	Quantum chemical electron impact mass spectrum prediction for de novo structure elucidation: Assessment against experimental reference data and comparison to competitive fragmentation modeling. *International Journal of Quantum Chemistry*, **2018**, 118, e25460	2.1	8
25	fragHAR: towards quantum-crystallographic X-ray structure refinement for polypeptides and proteins. *IUCrJ*, **2020**, 7, 158-165	4.7	7
24	Investigating the Resonance in Nitric Acid and the Nitrate Anion Based on a Modern Bonding Analysis. *Australian Journal of Chemistry*, **2018**, 71, 227	1.2	7
23	How does overcoordination create ion selectivity?. *Biophysical Chemistry*, **2013**, 172, 37-42	3.5	6
22	A theoretical study of the polarized neutron scattering from Cs3CoCl5. *Journal of Chemical Physics*, **2001**, 114, 2687-2697	3.9	6
21	Similarities and Differences between Crystal and Enzyme Environmental Effects on the Electron Density of Drug Molecules. *Chemistry - A European Journal*, **2021**, 27, 3407-3419	4.8	6
20	Implications of unitary invariance for gradient theory. *International Journal of Quantum Chemistry*, **1992**, 42, 445-458	2.1	5
19	Spatial symmetry and equivalence with unrestricted Hartree-Fock wavefunctions: application to the prediction of spin densities. *Molecular Physics*, **1997**, 92, 471-476	1.7	5
18	The quasirelativistic contact interaction and effective electron and spin densities at the nucleus: A model based on weighting the electron density with the finite Gaussian nucleus model. *Chemical Physics Letters*, **2013**, 580, 152-159	2.5	4
17	Ab initio study of the cyclic isomers of N2S4. *Chemical Physics*, **1995**, 198, 169-181	2.3	4
16	HgH meets relativistic quantum crystallography. How to teach relativity to a non-relativistic wavefunction. *Acta Crystallographica Section A: Foundations and Advances*, **2021**, 77, 54-66	1.7	4
15	Bridging Crystal Engineering and Drug Discovery by Utilizing Intermolecular Interactions and Molecular Shapes in Crystals. *Angewandte Chemie*, **2019**, 131, 16936-16940	3.6	3
14	Glycyl-L-alanine: a multi-temperature neutron study. *Acta Crystallographica Section C, Structural Chemistry*, **2014**, 70, 949-52	0.8	3
13	Contributions of the electronic spin and orbital current to the CoCl4(2-) magnetic field probed in polarised neutron diffraction experiments. *Journal of Chemical Physics*, **2012**, 137, 064107	3.9	3
12	The advanced treatment of hydrogen bonding in quantum crystallography. *Journal of Applied Crystallography*, **2021**, 54, 718-729	3.8	3
11	X-ray constrained wavefunctions based on Hirshfeld atoms. II. Reproducibility of electron densities in crystals of □-oxalic acid dihydrate. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2022**, 78, 397-415	1.8	3
10	X-ray constrained wavefunctions based on Hirshfeld atoms. I. Method and review. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2022**, 78, 312-332	1.8	3
9	Analytic SCF third and fourth derivatives with model potentials. *Chemical Physics Letters*, **1993**, 212, 18-26	2.5	2

8	Quantitative approaches to crystal engineering: applications to mechanical properties. *Acta Crystallographica Section A: Foundations and Advances*, **2017**, 73, C849-C849	1.7	2
7	Comment on "Inter/Intramolecular Bonds in TH (T = C/Si/Ge): H as Tetrel Bond Acceptor and the Uniqueness of Carbon Bonds". *Journal of Physical Chemistry A*, **2019**, 123, 9242-9243	2.8	1
6	Is it Reasonable to Obtain Information on the Polarizability and Hyperpolarizability Only from the Electron Density?. *Australian Journal of Chemistry*, **2018**, 71, 295	1.2	1
5	Using Wavefunctions to Get More Information Out of Diffraction Experiments **2011**, 213-257		1
4	Roby-Gould bond indices as a tool for understanding chemical bonding from a mathematical and quantum mechanical perspective. *Results in Chemistry*, **2020**, 2, 100053	2.1	0
3	X-ray wavefunction refinement Introduction, examples, validation. *Acta Crystallographica Section A: Foundations and Advances*, **2013**, 69, s589-s589		
2	Determination of Fluorophore Orientation and Energy Transfer from MD Simulations. *Biophysical Journal*, **2010**, 98, 582a	2.9	
1	Concerning the magnetisation density in magnetic neutron scattering experiments **2000**, 245-251		