Patrick Mccabe

List of Publications by Year
in descending order

35	21,264	394421 19	361022 35
papers	citations	h-index	g-index

35	35	35	18340
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Increasing the performance, trustworthiness and practical value of machine learning models: a case study predicting hydrogen bond network dimensionalities from molecular diagrams. CrystEngComm, 2020, 22, 7186-7192.	2.6	9
2	Mercury 4.0: from visualization to analysis, design and prediction. Journal of Applied Crystallography, 2020, 53, 226-235.	4.5	2,598
3	Note on Resonant and Non-resonant Peaks in Electron-Atom Total Scattering Cross Sections. Communications in Theoretical Physics, 2018, 69, 28.	2.5	1
4	Knowledge-Based Conformer Generation Using the Cambridge Structural Database. Journal of Chemical Information and Modeling, 2018, 58, 615-629.	5.4	47
5	Crystal structure prediction of flexible pharmaceutical-like molecules: density functional tight-binding as an intermediate optimisation method and for free energy estimation. Faraday Discussions, 2018, 211, 275-296.	3.2	29
6	Use of Crystal Structure Informatics for Defining the Conformational Space Needed for Predicting Crystal Structures of Pharmaceutical Molecules. Journal of Chemical Theory and Computation, 2017, 13, 5163-5171.	5.3	19
7	Near/far-side angular decompositions of Legendre polynomials using the amplitude-phase method. Journal of Mathematical Chemistry, 2017, 55, 1638-1648.	1.5	1
8	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	1.1	445
9	Generation of crystal structures using known crystal structures as analogues. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 530-541.	1.1	18
10	Knowledge-Based Optimization of Molecular Geometries Using Crystal Structures. Journal of Chemical Information and Modeling, 2016, 56, 652-661.	5.4	12
11	On Calculations of Legendre Functions and Associated Legendre Functions of the First Kind of Complex Degree. Communications in Theoretical Physics, 2015, 64, 9-12.	2.5	4
12	Partial-wave analysis of particular peaks in total scattering cross sections caused by a single partial wave. European Physical Journal D, 2014, 68, 1.	1.3	6
13	A theoretical study of spin-angular behaviors of potential scattering resonances. Physica Scripta, 2014, 89, 085401.	2.5	3
14	Kernel Density Estimation Applied to Bond Length, Bond Angle, and Torsion Angle Distributions. Journal of Chemical Information and Modeling, 2014, 54, 1284-1288.	5.4	12
15	Knowledge-Based Libraries for Predicting the Geometric Preferences of Druglike Molecules. Journal of Chemical Information and Modeling, 2014, 54, 2500-2514.	5.4	34
16	Bohr-Sommerfeld quantization condition for Dirac states derived from an Ermakov-type invariant. Journal of Mathematical Physics, 2013, 54, 052301.	1.1	1
17	Coupled radial SchrÃ¶dinger equations written as Dirac-type equations: application to an amplitude-phase approach. Journal of Physics A: Mathematical and Theoretical, 2012, 45, 135302.	2.1	2
18	The Ensemble Performance Index: An Improved Measure for Assessing Ensemble Pose Prediction Performance. Journal of Chemical Information and Modeling, 2011, 51, 2915-2919.	5.4	6

#	Article	IF	Citations
19	Amplitude-phase calculations of Regge poles obtained from coupled radial Dirac equations. Journal of Physics A: Mathematical and Theoretical, 2011, 44, 275305.	2.1	5
20	New software for statistical analysis of Cambridge Structural Database data. Journal of Applied Crystallography, 2011, 44, 882-886.	4.5	144
21	Intensive lowering of LDL cholesterol with 80 mg versus 20 mg simvastatin daily in 12â€˜064 survivors of myocardial infarction: a double-blind randomised trial. Lancet, The, 2010, 376, 1658-1669.	13.7	501
22	Mercury CSD 2.0â€“ new features for the visualization and investigation of crystal structures. Journal of Applied Crystallography, 2008, 41, 466-470.	4.5	7,887
23	Mercury: visualization and analysis of crystal structures. Journal of Applied Crystallography, 2006, 39, 453-457.	4.5	6,260
24	New software for searching the Cambridge Structural Database and visualizing crystal structures. Acta Crystallographica Section B: Structural Science, 2002, 58, 389-397.	1.8	2,791
25	Nearsideâ€“farside analysis of differential cross sections using Jacobi functions of the first and second kinds: Application to Ar+N2 rotationally inelastic scattering. Journal of Chemical Physics, 2001, 114, 5194-5206.	3.0	25
26	Nearsideâ€“farside analysis of state-selected differential cross sections for reactive molecular collisions. Physical Chemistry Chemical Physics, 1999, 1, 1115-1124.	2.8	75
27	Quantum scattering studies of spinâ€“orbit effects in the Cl(2P)+HClâ†’ClH+Cl(2P) reaction. Faraday Discussions, 1998, 110, 139-157.	3.2	54
28	Nearsideâ€“farside analysis of differential cross sections: Ar+N2 rotationally inelastic scattering using associated Legendre functions of the first and second kinds. Journal of Chemical Physics, 1998, 108, 5695-5703.	3.0	33
29	Coupled potential-energy surfaces and quantum reactive scattering for the Cl(2P)+HClâ†’ClH+Cl(2P) reaction. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 709-720.	1.7	65
30	Computation of Jacobi functions of the second kind for use in nearside-farside scattering theory. Journal of Computational and Applied Mathematics, 1997, 82, 447-464.	2.0	26
31	Nearsideâ€“farside analysis of differential cross sections: Diffraction and rainbow scattering in atomâ€“atom and atomâ€“molecule rotationally inelastic sudden collisions. Journal of Chemical Physics, 1996, 104, 2297-2311.	3.0	50
32	A theoretical study of the NH+NO reaction. Journal of Chemical Physics, 1995, 102, 6696-6705.	3.0	35
33	Nearsideâ€”farside analysis of angular scattering in elastic, inelastic and reactive molecular collisions. Chemical Physics Letters, 1993, 206, 119-122.	2.6	48
34	Complex angular momentum theory of molecular collisions: New phase rules for rotationally inelastic diffraction scattering in atomâ€“homonuclear diatomic molecule collisions. Journal of Chemical Physics, 1993, 98, 2947-2961.	3.0	12
35	Computational study of phase rules for rotationally inelastic diffraction scattering in atom-molecule collisions. Journal of Physics B: Atomic, Molecular and Optical Physics, 1991, 24, 2503-2519.	1.5	6