

# Patrick McCabe

## List of Publications by Year in descending order

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35  
papers

21,264  
citations

394421

19  
h-index

361022

35  
g-index

35  
all docs

35  
docs citations

35  
times ranked

18340  
citing authors

#	ARTICLE	IF	CITATIONS
1	<i>Mercury CSD 2.0</i> – new features for the visualization and investigation of crystal structures. <i>Journal of Applied Crystallography</i> , 2008, 41, 466-470.	4.5	7,887
2	<i>Mercury</i> : visualization and analysis of crystal structures. <i>Journal of Applied Crystallography</i> , 2006, 39, 453-457.	4.5	6,260
3	New software for searching the Cambridge Structural Database and visualizing crystal structures. <i>Acta Crystallographica Section B: Structural Science</i> , 2002, 58, 389-397.	1.8	2,791
4	<i>Mercury 4.0</i> : from visualization to analysis, design and prediction. <i>Journal of Applied Crystallography</i> , 2020, 53, 226-235.	4.5	2,598
5	Intensive lowering of LDL cholesterol with 80 mg versus 20 mg simvastatin daily in 12,064 survivors of myocardial infarction: a double-blind randomised trial. <i>Lancet</i> , 2010, 376, 1658-1669.	13.7	501
6	Report on the sixth blind test of organic crystal structure prediction methods. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 439-459.	1.1	445
7	New software for statistical analysis of Cambridge Structural Database data. <i>Journal of Applied Crystallography</i> , 2011, 44, 882-886.	4.5	144
8	Nearside-farside analysis of state-selected differential cross sections for reactive molecular collisions. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 1115-1124.	2.8	75
9	Coupled potential-energy surfaces and quantum reactive scattering for the $\text{Cl}(2P) + \text{HCl} \rightarrow \text{ClH} + \text{Cl}(2P)$ reaction. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1997, 93, 709-720.	1.7	65
10	Quantum scattering studies of spin-orbit effects in the $\text{Cl}(2P) + \text{HCl} \rightarrow \text{ClH} + \text{Cl}(2P)$ reaction. <i>Faraday Discussions</i> , 1998, 110, 139-157.	3.2	54
11	Nearside-farside analysis of differential cross sections: Diffraction and rainbow scattering in atom-atom and atom-molecule rotationally inelastic sudden collisions. <i>Journal of Chemical Physics</i> , 1996, 104, 2297-2311.	3.0	50
12	Nearside-farside analysis of angular scattering in elastic, inelastic and reactive molecular collisions. <i>Chemical Physics Letters</i> , 1993, 206, 119-122.	2.6	48
13	Knowledge-Based Conformer Generation Using the Cambridge Structural Database. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 615-629.	5.4	47
14	A theoretical study of the $\text{NH} + \text{NO}$ reaction. <i>Journal of Chemical Physics</i> , 1995, 102, 6696-6705.	3.0	35
15	Knowledge-Based Libraries for Predicting the Geometric Preferences of Druglike Molecules. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2500-2514.	5.4	34
16	Nearside-farside analysis of differential cross sections: $\text{Ar} + \text{N}_2$ rotationally inelastic scattering using associated Legendre functions of the first and second kinds. <i>Journal of Chemical Physics</i> , 1998, 108, 5695-5703.	3.0	33
17	Crystal structure prediction of flexible pharmaceutical-like molecules: density functional tight-binding as an intermediate optimisation method and for free energy estimation. <i>Faraday Discussions</i> , 2018, 211, 275-296.	3.2	29
18	Computation of Jacobi functions of the second kind for use in nearside-farside scattering theory. <i>Journal of Computational and Applied Mathematics</i> , 1997, 82, 447-464.	2.0	26

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19	Nearside/farside analysis of differential cross sections using Jacobi functions of the first and second kinds: Application to Ar+N <sub>2</sub> rotationally inelastic scattering. <i>Journal of Chemical Physics</i> , 2001, 114, 5194-5206.	3.0	25
20	Use of Crystal Structure Informatics for Defining the Conformational Space Needed for Predicting Crystal Structures of Pharmaceutical Molecules. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5163-5171.	5.3	19
21	Generation of crystal structures using known crystal structures as analogues. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 530-541.	1.1	18
22	Complex angular momentum theory of molecular collisions: New phase rules for rotationally inelastic diffraction scattering in atom-homonuclear diatomic molecule collisions. <i>Journal of Chemical Physics</i> , 1993, 98, 2947-2961.	3.0	12
23	Kernel Density Estimation Applied to Bond Length, Bond Angle, and Torsion Angle Distributions. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1284-1288.	5.4	12
24	Knowledge-Based Optimization of Molecular Geometries Using Crystal Structures. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 652-661.	5.4	12
25	Increasing the performance, trustworthiness and practical value of machine learning models: a case study predicting hydrogen bond network dimensionalities from molecular diagrams. <i>CrystEngComm</i> , 2020, 22, 7186-7192.	2.6	9
26	Computational study of phase rules for rotationally inelastic diffraction scattering in atom-molecule collisions. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 1991, 24, 2503-2519.	1.5	6
27	The Ensemble Performance Index: An Improved Measure for Assessing Ensemble Pose Prediction Performance. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 2915-2919.	5.4	6
28	Partial-wave analysis of particular peaks in total scattering cross sections caused by a single partial wave. <i>European Physical Journal D</i> , 2014, 68, 1.	1.3	6
29	Amplitude-phase calculations of Regge poles obtained from coupled radial Dirac equations. <i>Journal of Physics A: Mathematical and Theoretical</i> , 2011, 44, 275305.	2.1	5
30	On Calculations of Legendre Functions and Associated Legendre Functions of the First Kind of Complex Degree. <i>Communications in Theoretical Physics</i> , 2015, 64, 9-12.	2.5	4
31	A theoretical study of spin-angular behaviors of potential scattering resonances. <i>Physica Scripta</i> , 2014, 89, 085401.	2.5	3
32	Coupled radial Schrödinger equations written as Dirac-type equations: application to an amplitude-phase approach. <i>Journal of Physics A: Mathematical and Theoretical</i> , 2012, 45, 135302.	2.1	2
33	Bohr-Sommerfeld quantization condition for Dirac states derived from an Ermakov-type invariant. <i>Journal of Mathematical Physics</i> , 2013, 54, 052301.	1.1	1
34	Near/far-side angular decompositions of Legendre polynomials using the amplitude-phase method. <i>Journal of Mathematical Chemistry</i> , 2017, 55, 1638-1648.	1.5	1
35	Note on Resonant and Non-resonant Peaks in Electron-Atom Total Scattering Cross Sections. <i>Communications in Theoretical Physics</i> , 2018, 69, 28.	2.5	1