

# C M Hoffmann

## List of Publications by Year in descending order

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57  
papers

1,930  
citations

236925

25  
h-index

254184

43  
g-index

65  
all docs

65  
docs citations

65  
times ranked

3329  
citing authors

#	ARTICLE	IF	CITATIONS
1	Synthesis and Structure Characterization of Copper Terephthalate Metal-Organic Frameworks. European Journal of Inorganic Chemistry, 2009, 2009, 2338-2343.	2.0	312
2	Quantitative analysis of intermolecular interactions in orthorhombic rubrene. IUCr, 2015, 2, 563-574.	2.2	206
3	Heterolytic Cleavage of Hydrogen by an Iron Hydrogenase Model: An Fe-N Dihydrogen Bond Characterized by Neutron Diffraction. Angewandte Chemie - International Edition, 2014, 53, 5300-5304.	13.8	102
4	Synthesis and Reactivity of Tethered 1,6-(Phosphinoarene)ruthenium Dichlorides. Organometallics, 1998, 17, 330-337.	2.3	86
5	Integration of neutron time-of-flight single-crystal Bragg peaks in reciprocal space. Journal of Applied Crystallography, 2014, 47, 915-921.	4.5	82
6	CrystalPlan: an experiment-planning tool for crystallography. Journal of Applied Crystallography, 2011, 44, 418-423.	4.5	67
7	The macromolecular neutron diffractometer (MaNDi) at the Spallation Neutron Source, Oak Ridge: enhanced optics design, high-resolution neutron detectors and simulated diffraction. Journal of Applied Crystallography, 2010, 43, 570-577.	4.5	64
8	Anharmonicity and atomic distribution of SnTe and PbTe thermoelectrics. Physical Review B, 2014, 90, .	3.2	64
9	Weyl-mediated helical magnetism in NdAlSi. Nature Materials, 2021, 20, 1650-1656.	27.5	48
10	Reciprocal Salt Flux Growth of LiFePO <sub>4</sub> Single Crystals with Controlled Defect Concentrations. Chemistry of Materials, 2013, 25, 4574-4584.	6.7	43
11	A suite-level review of the neutron single-crystal diffraction instruments at Oak Ridge National Laboratory. Review of Scientific Instruments, 2018, 89, 092802.	1.3	43
12	Structure symmetry determination and magnetic evolution in Sr <sub>2</sub> Ir <sub>1-x</sub> Rh <sub>x</sub> O <sub>4</sub> . Physical Review B, 2015, 92, .	3.2	42
13	Clinotobermorite, Ca <sub>5</sub> [Si <sub>3</sub> O <sub>8</sub> (OH)] <sub>2</sub> · 4 H <sub>2</sub> O p=n- Ca <sub>5</sub> [Si <sub>6</sub> O <sub>17</sub> ] · 5 H <sub>2</sub> O, a natural Cp=n-Sp=n-H(l) type cement mineral: determination of the substructure. Zeitschrift Fur Kristallographie - Crystalline Materials, 1997, 212, 864-873.	0.8	41
14	On the Chemistry and Physical Properties of Flux and Floating Zone Grown SmB <sub>6</sub> Single Crystals. Scientific Reports, 2016, 6, 20860.	3.3	38
15	Thermodynamic and kinetic studies of H <sub>2</sub> and N <sub>2</sub> binding to bimetallic nickel-group 13 complexes and neutron structure of a Ni(η <sup>2</sup> -H <sub>2</sub> ) adduct. Chemical Science, 2019, 10, 7029-7042.	7.4	38
16	Solution <sup>31</sup> P NMR Study of the Acid-Catalyzed Formation of a Highly Charged {U <sub>24</sub> Pp <sub>12</sub> } Nanocluster, [(UO <sub>2</sub> ) <sub>24</sub> (O <sub>2</sub> ) <sub>24</sub> (P <sub>2</sub> O <sub>7</sub> ) <sub>12</sub> ] <sup>48-</sup> and Its Structural Characterization in the Solid State Using Single-Crystal Neutron Diffraction. Journal of the American Chemical Society, 2016, 138, 8547-8553.	18.4	35
17	Expanding Lorentz and spectrum corrections to large volumes of reciprocal space for single-crystal time-of-flight neutron diffraction. Journal of Applied Crystallography, 2016, 49, 497-506.	4.5	34
18	Test of a continuously polarized <sup>3</sup> He neutron spin filter with NMR-based polarization inversion on a single-crystal diffractometer. Physica B: Condensed Matter, 2006, 385-386, 1131-1133.	2.7	33

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19	Free H <sub>2</sub> Rotation vs Jahn-Teller Constraints in the Nonclassical Trigonal (TPB)CoH <sub>2</sub> Complex. Journal of the American Chemical Society, 2014, 136, 14998-15009.	13.7	33
20	Microdomain dynamics in single-crystal BaTiO <sub>3</sub> during paraelectric-ferroelectric phase transition measured with time-of-flight neutron scattering. Physical Review B, 2015, 92, .	3.2	32
21	and universal behavior in quantum spin liquid candidates synthetic barlowite and herbertsmithite. Physical Review Materials, 2018, 2, .	2.4	31
22	High-resolution neutron crystallographic studies of the hydration of the coenzyme cob(II)alamin. Acta Crystallographica Section D: Biological Crystallography, 2011, 67, 584-591.	2.5	30
23	Structural modulations and magnetic properties of off-stoichiometric Ni-Mn-Ga magnetic shape memory alloys. Physical Review B, 2012, 85, .	3.2	30
24	Orthorhombic Jahn-Teller distortion and Si-OH in mozartite, CaMn (super 3+) O[SiO <sub>3</sub> OH]; a single-crystal X-ray, FTIR, and structure modeling study. American Mineralogist, 1997, 82, 841-848.	1.9	29
25	Soft antiphase tilt of oxygen octahedra in the hybrid improper multiferroic CaMn <sub>3</sub> O <sub>7</sub> . Physical Review B, 2018, 97, .	3.2	27
26	Crystal chemistry and optics of bazzite from Furkabasistunnel (Switzerland). Mineralogy and Petrology, 1995, 52, 113-126.	1.1	24
27	Spectroscopic Studies of the Magnetic Excitation and Spin-Phonon Couplings in a Single-Molecule Magnet. Chemistry - A European Journal, 2019, 25, 15846-15857.	3.3	22
28	Quantitative analysis of hydrogen sites and occupancy in deep mantle hydrous wadsleyite using single crystal neutron diffraction. Scientific Reports, 2016, 6, 34988.	3.3	21
29	Spin density in YTiO <sub>3</sub> : I. Joint refinement of polarized neutron diffraction and magnetic x-ray diffraction data leading to insights into orbital ordering. Physical Review B, 2017, 96, .	3.2	20
30	Next-generation diamond cell and applications to single-crystal neutron diffraction. Review of Scientific Instruments, 2018, 89, 092902.	1.3	20
31	Self-assembly of molecular ions via like-charge ion interactions and through-space defined organic domains. Chemical Communications, 2017, 53, 10934-10937.	4.1	19
32	Continuously operating compact He-based neutron spin filter. Physica B: Condensed Matter, 2005, 356, 86-90.	2.7	17
33	Comparison of different strategies for modelling hydrogen atoms in charge density analyses. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 434-441.	1.1	17
34	Nonequilibrium orbital transitions via applied electrical current in calcium ruthenates. Physical Review B, 2019, 100, .	3.2	17
35	Analyzing diffuse scattering with supercomputers. Journal of Applied Crystallography, 2013, 46, 1616-1625.	4.5	12
36	Accurate atomic displacement parameters from time-of-flight neutron-diffraction data at TOPAZ. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, 679-681.	0.1	12

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37	Intermolecular Interactions in Solid-State Metalloporphyrins and Their Impacts on Crystal and Molecular Structures. <i>Inorganic Chemistry</i> , 2014, 53, 11552-11562.	4.0	11
38	Determination of hydrogen site and occupancy in hydrous Mg <sub>2</sub> SiO <sub>4</sub> spinel by single-crystal neutron diffraction. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2018, 74, 115-120.	1.1	11
39	Fast Rotational Diffusion of Water Molecules in a 2D Hydrogen Bond Network at Cryogenic Temperatures. <i>Physical Review Letters</i> , 2018, 120, 196001.	7.8	10
40	Exotic Magnetic Field-Induced Spin-Superstructures in a Mixed Honeycomb-Triangular Lattice System. <i>Physical Review X</i> , 2019, 9, .	8.9	10
41	LiCa <sub>3</sub> As <sub>2</sub> H and Ca <sub>14</sub> As <sub>6</sub> X <sub>7</sub> (X = C, H, N): Two New Arsenide Hydride Phases Grown from Ca/Li Metal Flux. <i>Inorganic Chemistry</i> , 2014, 53, 10620-10626.	4.0	9
42	From the source: student-centred guest lecturing in a chemical crystallography class. <i>Journal of Applied Crystallography</i> , 2018, 51, 909-914.	4.5	9
43	Nanoscale Atomic Displacements Ordering for Enhanced Piezoelectric Properties in Lead-Free ABO <sub>3</sub> Ferroelectrics. <i>Advanced Materials</i> , 2015, 27, 4330-4335.	21.0	8
44	The neutron diffraction structure of [Ir <sub>4</sub> (IME) <sub>8</sub> H <sub>10</sub> ] <sub>2</sub> <sup>+</sup> polyhydride cluster: Testing the computational hydride positional assignments. <i>Journal of Organometallic Chemistry</i> , 2017, 849-850, 17-21.	1.8	8
45	Pseudospin-lattice coupling and electric control of the square-lattice iridate Sr <sub>2</sub> IrO <sub>4</sub> . <i>Physical Review B</i> , 2020, 102, .	3.2	7
46	K-space algorithmic reconstruction (KAREN): a robust statistical methodology to separate Bragg and diffuse scattering. <i>Journal of Applied Crystallography</i> , 2020, 53, 159-169.	4.5	7
47	Time filtering of event based neutron scattering data: A pathway to study the dynamic structural responses of materials. <i>Review of Scientific Instruments</i> , 2018, 89, 092803.	1.3	6
48	Strong hydrogen bonding in a dense hydrous magnesium silicate discovered by neutron Laue diffraction. <i>IUCr</i> , 2020, 7, 370-374.	2.2	6
49	Synthesis, Structure, and Physical Properties of Ln(Cu,Al,Ga) <sub>13</sub> (Ln = La, Pr, and Eu) and Eu(Cu,Al) <sub>13</sub> . <i>Inorganic Chemistry</i> , 2012, 51, 10193-10202.	4.0	5
50	Probing orientation information using 3-dimensional reciprocal space volume analysis. <i>Review of Scientific Instruments</i> , 2019, 90, 013902.	1.3	5
51	4,4'-Dinitro-2,2'-bipyridine. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 1997, 53, 1719-1721.	0.4	4
52	Neutron and X-ray investigations of the Jahn-Teller switch in partially deuterated ammonium copper Tutton salt, (NH <sub>4</sub> ) <sub>2</sub> [Cu(H <sub>2</sub> O) <sub>6</sub> ](SO <sub>4</sub> ) <sub>2</sub> . <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2017, 73, 87-93.	1.1	3
53	Initial testing of a Compact Crystal Positioning System for the TOPAZ Single-Crystal Diffractometer at the Spallation Neutron Source. <i>Journal of Physics: Conference Series</i> , 2010, 251, 012084.	0.4	2
54	<i>Operando</i> single crystal neutron diffraction reveals insight into the field response mechanisms in the hydrogen-bonded KH <sub>2</sub> PO <sub>4</sub> ferroelectric. <i>APL Materials</i> , 2021, 9, .	5.1	1

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55	Frontispiece: Heterolytic Cleavage of Hydrogen by an Iron Hydrogenase Model: An Fe-Hâ€¦â€¦â€¦H-N Dihydrogen Bond Characterized by Neutron Diffraction. <i>Angewandte Chemie - International Edition</i> , 2014, 53, n/a-n/a.	13.8	0
56	Frontispiz: Heterolytic Cleavage of Hydrogen by an Iron Hydrogenase Model: An Fe-Hâ€¦â€¦â€¦H-N Dihydrogen Bond Characterized by Neutron Diffraction. <i>Angewandte Chemie</i> , 2014, 126, n/a-n/a.	2.0	0
57	Ferroelectric Materials: Nanoscale Atomic Displacements Ordering for Enhanced Piezoelectric Properties in Lead-Free ABO <sub>3</sub> Ferroelectrics ( <i>Adv. Mater.</i> 29/2015). <i>Advanced Materials</i> , 2015, 27, 4329-4329.	21.0	0