

# 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  | <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         |
| 2  | Weyl-mediated helical magnetism in NdAlSi. <i>Nature Materials</i> , 2021, 20, 1650-1656.  | 27.5 | 48        |
| 3  | 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         |
| 4  | Strong hydrogen bonding in a dense hydrous magnesium silicate discovered by neutron Laue diffraction. <i>IUCr</i> , 2020, 7, 370-374.  | 2.2  | 6         |
| 5  | 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         |
| 6  | Spectroscopic Studies of the Magnetic Excitation and Spin-Phonon Couplings in a Single-Molecule Magnet. <i>Chemistry - A European Journal</i> , 2019, 25, 15846-15857.   | 3.3  | 22        |
| 7  | 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(μ <sup>2</sup> -H <sub>2</sub> ) adduct. <i>Chemical Science</i> , 2019, 10, 7029-7042.               | 7.4  | 38        |
| 8  | Exotic Magnetic Field-Induced Spin-Superstructures in a Mixed Honeycomb-Triangular Lattice System. <i>Physical Review X</i> , 2019, 9, .   | 8.9  | 10        |
| 9  | Comparison of different strategies for modelling hydrogen atoms in charge density analyses. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2019, 75, 434-441.  | 1.1  | 17        |
| 10 | Nonequilibrium orbital transitions via applied electrical current in calcium ruthenates. <i>Physical Review B</i> , 2019, 100, .   | 3.2  | 17        |
| 11 | Probing orientation information using 3-dimensional reciprocal space volume analysis. <i>Review of Scientific Instruments</i> , 2019, 90, 013902.  | 1.3  | 5         |
| 12 | Soft antiphase tilt of oxygen octahedra in the hybrid improper multiferroic $\text{CaO}_7\text{Mn}_3$ . <i>Physical Review B</i> , 2018, 97, .   | 3.2  | 27        |
| 13 | A suite-level review of the neutron single-crystal diffraction instruments at Oak Ridge National Laboratory. <i>Review of Scientific Instruments</i> , 2018, 89, 092802.   | 1.3  | 43        |
| 14 | 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        |
| 15 | Next-generation diamond cell and applications to single-crystal neutron diffraction. <i>Review of Scientific Instruments</i> , 2018, 89, 092902.   | 1.3  | 20        |
| 16 | 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         |
| 17 | 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         |
| 18 | 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        |

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|----|--|------|-----------|
| 19 | Single-crystal growth of $\text{Cu}_4\text{O}(\text{NH}_4)_2(\text{SO}_4)_2$ and universal behavior in quantum spin liquid candidates synthetic barlowite and herbertsmithite. 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> . Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 87-93. | 2.4  | 31        |
| 20 | The neutron diffraction structure of [Ir <sub>4</sub> (IME) <sub>8</sub> H <sub>10</sub> ] <sub>2+</sub> polyhydride cluster: Testing the computational hydride positional assignments. Journal of Organometallic Chemistry, 2017, 849-850, 17-21.   | 1.1  | 3         |
| 21 | Self-assembly of molecular ions via like-charge ion interactions and through-space defined organic domains. Chemical Communications, 2017, 53, 10934-10937.  | 1.8  | 8         |
| 22 | Spin density in $\text{YTiO}_3$ : I. Joint refinement of polarized neutron diffraction and magnetic x-ray diffraction data leading to insights into orbital ordering. Physical Review B, 2017, 96, .   | 4.1  | 19        |
| 23 | 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.  | 3.2  | 20        |
| 24 | Quantitative analysis of hydrogen sites and occupancy in deep mantle hydrous wadsleyite using single crystal neutron diffraction. Scientific Reports, 2016, 6, 34988.  | 4.5  | 34        |
| 25 | 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  | 21        |
| 26 | 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.   | 3.3  | 38        |
| 27 | Ferroelectric Materials: Nanoscale Atomic Displacements Ordering for Enhanced Piezoelectric Properties in Lead-Free ABO <sub>3</sub> Ferroelectrics (Adv. Mater. 29/2015). Advanced Materials, 2015, 27, 4329-4329.  | 4.8  | 0         |
| 28 | Microdomain dynamics in single-crystal $\text{BaTiO}_3$ during paraelectric-ferroelectric phase transition measured with time-of-flight neutron scattering. Physical Review B, 2015, 92, .   | 3.2  | 32        |
| 29 | Structure symmetry determination and magnetic evolution in $\text{Sr}_2\text{Ir}_2\text{Rh}_2\text{O}_4$ . Physical Review B, 2015, 92, .  | 3.2  | 42        |
| 30 | Nanoscale Atomic Displacements Ordering for Enhanced Piezoelectric Properties in Lead-Free ABO <sub>3</sub> Ferroelectrics. Advanced Materials, 2015, 27, 4330-4335.   | 21.0 | 8         |
| 31 | Quantitative analysis of intermolecular interactions in orthorhombic rubrene. IUCr, 2015, 2, 563-574.  | 2.2  | 206       |
| 32 | Anharmonicity and atomic distribution of SnTe and PbTe thermoelectrics. Physical Review B, 2014, 90, .   | 3.2  | 64        |
| 33 | 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        |
| 34 | Heterolytic Cleavage of Hydrogen by an Iron Hydrogenase Model: An Fe-H-N Dihydrogen Bond Characterized by Neutron Diffraction. Angewandte Chemie - International Edition, 2014, 53, 5300-5304.   | 13.8 | 102       |
| 35 | Frontispiece: Heterolytic Cleavage of Hydrogen by an Iron Hydrogenase Model: An Fe-H-N Dihydrogen Bond Characterized by Neutron Diffraction. Angewandte Chemie - International Edition, 2014, 53, n/a-n/a.   | 13.8 | 0         |

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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 | Free H <sub>2</sub> Rotation vs Jahn-Teller Constraints in the Nonclassical Trigonal (TPB)CoH <sub>2</sub> Complex. <i>Journal of the American Chemical Society</i> , 2014, 136, 14998-15009.  | 13.7 | 33        |
| 39 | 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         |
| 40 | Integration of neutron time-of-flight single-crystal Bragg peaks in reciprocal space. <i>Journal of Applied Crystallography</i> , 2014, 47, 915-921.   | 4.5  | 82        |
| 41 | Frontispiz: Heterolytic Cleavage of Hydrogen by an Iron Hydrogenase Model: An Fe-H...H-N Dihydrogen Bond Characterized by Neutron Diffraction. <i>Angewandte Chemie</i> , 2014, 126, n/a-n/a.  | 2.0  | 0         |
| 42 | Analyzing diffuse scattering with supercomputers. <i>Journal of Applied Crystallography</i> , 2013, 46, 1616-1625.   | 4.5  | 12        |
| 43 | Reciprocal Salt Flux Growth of LiFePO <sub>4</sub> Single Crystals with Controlled Defect Concentrations. <i>Chemistry of Materials</i> , 2013, 25, 4574-4584.   | 6.7  | 43        |
| 44 | Synthesis, Structure, and Physical Properties of Ln(Cu,Al,Ga) <sub>13</sub> x (Ln= La, Pr, and Eu) and Eu(Cu,Al) <sub>13</sub> x. <i>Inorganic Chemistry</i> , 2012, 51, 10193-10202.  | 4.0  | 5         |
| 45 | Structural modulations and magnetic properties of off-stoichiometric Ni-Mn-Ga magnetic shape memory alloys. <i>Physical Review B</i> , 2012, 85, .   | 3.2  | 30        |
| 46 | CrystalPlan: an experiment-planning tool for crystallography. <i>Journal of Applied Crystallography</i> , 2011, 44, 418-423.   | 4.5  | 67        |
| 47 | High-resolution neutron crystallographic studies of the hydration of the coenzyme cob(II)alamin. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011, 67, 584-591.  | 2.5  | 30        |
| 48 | 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         |
| 49 | The macromolecular neutron diffractometer (MaNDi) at the Spallation Neutron Source, Oak Ridge: enhanced optics design, high-resolution neutron detectors and simulated diffraction. <i>Journal of Applied Crystallography</i> , 2010, 43, 570-577.   | 4.5  | 64        |
| 50 | Synthesis and Structure Characterization of Copper Terephthalate Metal-Organic Frameworks. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 2338-2343.   | 2.0  | 312       |
| 51 | Test of a continuously polarized <sup>3</sup> He neutron spin filter with NMR-based polarization inversion on a single-crystal diffractometer. <i>Physica B: Condensed Matter</i> , 2006, 385-386, 1131-1133.  | 2.7  | 33        |
| 52 | Continuously operating compact He-based neutron spin filter. <i>Physica B: Condensed Matter</i> , 2005, 356, 86-90.  | 2.7  | 17        |
| 53 | Synthesis and Reactivity of Tethered 1:1:6-(Phosphinoarene)ruthenium Dichlorides. <i>Organometallics</i> , 1998, 17, 330-337.  | 2.3  | 86        |
| 54 | 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. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 1997, 212, 864-873. | 0.8  | 41        |

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|----|---|-----|-----------|
| 55 | 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. <i>American Mineralogist</i> , 1997, 82, 841-848. | 1.9 | 29        |
| 56 | 4,4'-Dinitro-2,2'-bipyridine. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 1997, 53, 1719-1721.  | 0.4 | 4         |
| 57 | Crystal chemistry and optics of bazzite from Furkabisstunnel (Switzerland). <i>Mineralogy and Petrology</i> , 1995, 52, 113-126.  | 1.1 | 24        |