# Jacqueline M Cole

List of Publications by Year
in descending order



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|---|---|---|---|
| 149 papers | 5,779 citations | 94415 37 h-index | 88628 70 g-index |
| 151 all docs | 151 docs citations | 151 times ranked | 6420 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Anchoring Groups for Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2015, 7, 3427-3455. | 8.0 | 654 |
| 2 | Black silicon: fabrication methods, properties and solar energy applications. Energy and Environmental Science, 2014, 7, 3223-3263. | 30.8 | 396 |
| 3 | ChemDataExtractor: A Toolkit for Automated Extraction of Chemical Information from the Scientific Literature. Journal of Chemical Information and Modeling, 2016, 56, 1894-1904. | 5.4 | 297 |
| 4 | Molecular Origins of Optoelectronic Properties in Coumarin Dyes: Toward Designer Solar Cell and Laser Applications. Journal of Physical Chemistry A, 2012, 116, 727-737. | 2.5 | 244 |
| 5 | Dye aggregation in dye-sensitized solar cells. Journal of Materials Chemistry A, 2017, 5, 19541-19559. | 10.3 | 240 |
| 6 | Molecular Design of UVâ€“vis Absorption and Emission Properties in Organic Fluorophores: Toward Larger Bathochromic Shifts, Enhanced Molar Extinction Coefficients, and Greater Stokes Shifts. Journal of Physical Chemistry C, 2013, 117, 16584-16595. | 3.1 | 209 |
| 7 | Cosensitization in Dye-Sensitized Solar Cells. Chemical Reviews, 2019, 119, 7279-7327. | 47.7 | 190 |
| 8 | Data-driven materials research enabled by natural language processing and information extraction. Applied Physics Reviews, 2020, 7, . | 11.3 | 117 |
| 9 | Light-Induced Metastable Linkage Isomers of Ruthenium Sulfur Dioxide Complexes. Inorganic Chemistry, 2003, 42, 140-147. | 4.0 | 105 |
| 10 | Solvent Effects on the UVâ€“vis Absorption and Emission of Optoelectronic Coumarins: a Comparison of Three Empirical Solvatochromic Models. Journal of Physical Chemistry C, 2013, 117, 14731-14741. | 3.1 | 98 |
| 11 | Variation in Optoelectronic Properties of Azo Dye-Sensitized TiO<sub>2</sub> Semiconductor Interfaces with Different Adsorption Anchors: Carboxylate, Sulfonate, Hydroxyl and Pyridyl Groups. ACS Applied Materials & Interfaces, 2014, 6, 7535-7546. | 8.0 | 95 |
| 12 | Auto-generated materials database of Curie and NÃ©el temperatures via semi-supervised relationship extraction. Scientific Data, 2018, 5, 180111. | 5.3 | 84 |
| 13 | Relating Electron Donor and Carboxylic Acid Anchoring Substitution Effects in Azo Dyes to Dye-Sensitized Solar Cell Performance. ACS Sustainable Chemistry and Engineering, 2013, 1, 1440-1452. | 6.7 | 83 |
| 14 | Neutron and X-ray Diffraction and Spectroscopic Investigations of Intramolecular [Cï£¿Hâ‹…â‹…â‹…Fï£¿C] Contacts in Post-Metallocene Polyolefin Catalysts: Modeling Weak Attractive Polymerâ€“Ligand Interactions. Chemistry - A European Journal, 2006, 12, 2607-2619. | 3.3 | 82 |
| 15 | Single-crystal X-ray diffraction studies of photo-induced molecular species. Chemical Society Reviews, 2004, 33, 501. | 38.1 | 81 |
| 16 | Photocrystallographic structure determination of a new geometric isomer of [Ru(NH3)4(H2O)(î·1-OSO)][MeC6H4SO3]2. Chemical Communications, 2006, , 2448-2450. | 4.1 | 78 |
| 17 | A database of battery materials auto-generated using ChemDataExtractor. Scientific Data, 2020, 7, 260. | 5.3 | 76 |
| 18 | Organic materials for second-harmonic generation: advances in relating structure to function. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2003, 361, 2751-2770. | 3.4 | 69 |

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| 19 | Photocrystallography. Acta Crystallographica Section A: Foundations and Advances, 2008, 64, 259-271. | 0.3 | 63 |
| 20 | Comparative dataset of experimental and computational attributes of UV/vis absorption spectra. Scientific Data, 2019, 6, 307. | 5.3 | 63 |
| 21 | A Design-to-Device Pipeline for Data-Driven Materials Discovery. Accounts of Chemical Research, 2020, 53, 599-610. | 15.6 | 59 |
| 22 | An x-ray diffraction and31P MAS NMR study of rare-earth phosphate glasses, (R2O3)x(P2O5)1-x,x= 0.175-0.263, R = La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er. Journal of Physics Condensed Matter, 2001, 13, 4105-4122. | 1.8 | 58 |
| 23 | Magnetic and superconducting phase diagrams and transition temperatures predicted using text mining and machine learning. Npj Computational Materials, 2020, 6, . | 8.7 | 58 |
| 24 | Photoconversion Bonding Mechanism in Ruthenium Sulfur Dioxide Linkage Photoisomers Revealed by in Situ Diffraction. Journal of the American Chemical Society, 2012, 134, 11860-11863. | 13.7 | 56 |
| 25 | Data mining with molecular design rules identifies new class of dyes for dye-sensitised solar cells. Physical Chemistry Chemical Physics, 2014, 16, 26684-26690. | 2.8 | 55 |
| 26 | Substantial Intramolecular Charge Transfer Induces Long Emission Wavelengths and Mega Stokes Shifts in 6-Aminocoumarins. Journal of Physical Chemistry C, 2017, 121, 13274-13279. | 3.1 | 55 |
| 27 | 3-D Inorganic Crystal Structure Generation and Property Prediction via Representation Learning. Journal of Chemical Information and Modeling, 2020, 60, 4518-4535. | 5.4 | 50 |
| 28 | Ruâ€“OSO Coordination Photogenerated at 100 K in Tetraammineaqua(sulfur dioxide)ruthenium(II) (Â±)-Camphorsulfonate. Inorganic Chemistry, 2012, 51, 1204-1206. | 4.0 | 44 |
| 29 | On the accuracy of density functional theory and wave function methods for calculating vertical ionization energies. Journal of Chemical Physics, 2015, 142, 194114. | 3.0 | 44 |
| 30 | Molecular Origins of Dye Aggregation and Complex Formation Effects in Coumarin 343. Journal of Physical Chemistry C, 2013, 117, 14723-14730. | 3.1 | 43 |
| 31 | TiO<sub>2</sub>-Assisted Photoisomerization of Azo Dyes Using Self-Assembled Monolayers: Case Study on para-Methyl Red Towards Solar-Cell Applications. ACS Applied Materials & Interfaces, 2014, 6, 3742-3749. | 8.0 | 43 |
| 32 | ChemDataExtractor 2.0: Autopopulated Ontologies for Materials Science. Journal of Chemical Information and Modeling, 2021, 61, 4280-4289. | 5.4 | 43 |
| 33 | Influence of hydrogen bonding on the second harmonic generation effect: neutron diffraction study of 4-nitro-4â€²-methylbenzylidene aniline. Acta Crystallographica Section B: Structural Science, 2001, 57, 410-414. | 1.8 | 42 |
| 34 | A new polymorph of terpyridine: variable temperature X-ray diffraction studies and solid state photophysical properties. CrystEngComm, 2005, 7, 269. | 2.6 | 42 |
| 35 | Adsorption Properties of p-Methyl Red Monomeric-to-Pentameric Dye Aggregates on Anatase (101) Titania Surfaces: First-Principles Calculations of Dye/TiO<sub>2</sub> Photoanode Interfaces for Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2014, 6, 15760-15766. | 8.0 | 42 |
| 36 | Charge-density study of the nonlinear optical precursor DED-TCNQ at 20 K. Physical Review B, 2002, 65, . | 3.2 | 41 |

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| 37 | Effects of the reaction cavity on metastable optical excitation in ruthenium-sulfur dioxide complexes. Physical Review B, 2010, 82, . | 3.2 | 41 |
| 38 | Designâ€toâ€Device Approach Affords Panchromatic Coâ€Sensitized Solar Cells. Advanced Energy Materials, 2019, 9, 1802820. | 19.5 | 40 |
| 39 | Conformational variability of molecules in different crystal environments: a database study. Acta Crystallographica Section B: Structural Science, 2008, 64, 348-362. | 1.8 | 36 |
| 40 | Molecular Origins of Optoelectronic Properties in Coumarins 343, 314T, 445, and 522B. Journal of Physical Chemistry C, 2013, 117, 14130-14141. | 3.1 | 36 |
| 41 | Rational Design of Dithienopicenocarbazole-Based Dyes and a Prediction of Their Energy-Conversion Efficiency Characteristics for Dye-Sensitized Solar Cells. ACS Applied Energy Materials, 2018, 1, 1435-1444. | 5.1 | 36 |
| 42 | Tuning Solvatochromism of Azo Dyes with Intramolecular Hydrogen Bonding in Solution and on Titanium Dioxide Nanoparticles. Journal of Physical Chemistry C, 2013, 117, 26316-26323. | 3.1 | 35 |
| 43 | Removal or storage of environmental pollutants and alternative fuel sources with inorganic adsorbents via hostâ€“guest encapsulation. Journal of Materials Chemistry A, 2017, 5, 10746-10771. | 10.3 | 35 |
| 44 | Molecular Origins of the High-Performance Nonlinear Optical Susceptibility in a Phenolic Polyene Chromophore: Electron Density Distributions, Hydrogen Bonding, and ab Initio Calculations. Journal of Physical Chemistry C, 2013, 117, 9416-9430. | 3.1 | 34 |
| 45 | X-ray and neutron diffraction studies of the non-linear optical compounds MBANP and MBADNP at 20â€…K: charge-density and hydrogen-bonding analyses. Acta Crystallographica Section B: Structural Science, 2002, 58, 690-700. | 1.8 | 33 |
| 46 | Modulation of N3 and N719 dyeÂ·Â·Â·TiO<sub>2</sub> Interfacial Structures in Dye-Sensitized Solar Cells As Influenced by Dye Counter Ions, Dye Deprotonation Levels, and Sensitizing Solvent. ACS Applied Energy Materials, 2018, 1, 2821-2831. | 5.1 | 31 |
| 47 | A new form of analytical chemistry: distinguishing the molecular structure of photo-induced states from ground-states. Analyst, The, 2011, 136, 448-455. | 3.5 | 30 |
| 48 | Modeling electron density distributions from X-ray diffraction to derive optical properties: Constrained wavefunction versus multipole refinement. Journal of Chemical Physics, 2013, 139, 064108. | 3.0 | 30 |
| 49 | A rare-earth K-edge EXAFS study of rare-earth phosphate glasses, (R2O3)x(P2O5)1-x,x= 0.187-0.239, R = La, Nd, Sm, Eu, Gd, Dy, Er. Journal of Physics Condensed Matter, 2001, 13, 6659-6674. | 1.8 | 29 |
| 50 | Dye Aggregation and Complex Formation Effects in 7-(Diethylamino)-coumarin-3-carboxylic Acid. Journal of Physical Chemistry C, 2014, 118, 13042-13051. | 3.1 | 29 |
| 51 | ImageDataExtractor: A Tool To Extract and Quantify Data from Microscopy Images. Journal of Chemical Information and Modeling, 2020, 60, 2492-2509. | 5.4 | 29 |
| 52 | Can nitro groups really anchor onto TiO<sub>2</sub>? Case study of dye-to-TiO<sub>2</sub>adsorption using azo dyes with NO<sub>2</sub>substituents. Physical Chemistry Chemical Physics, 2016, 18, 19062-19069. | 2.8 | 28 |
| 53 | A neutron diffraction and27Al MQMAS NMR study of rare-earth phosphate glasses, (R2O3)x(P2O5)1-x,x= 0.187-0.263, R = Ce, Nd, Tb containing Al impurities. Journal of Physics Condensed Matter, 1999, 11, 9165-9178. | 1.8 | 27 |
| 54 | Preferred Molecular Orientation of Coumarin 343 on TiO<sub>2</sub> Surfaces: Application to Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2015, 7, 16404-16409. | 8.0 | 27 |

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| 55 | Light-Induced Macroscopic Peeling of Single Crystal Driven by Photoisomeric Nano-Optical Switching. Chemistry of Materials, 2019, 31, 4927-4935. | 6.7 | 27 |
| 56 | Rationalizing the molecular origins of Ru- and Fe-based dyes for dye-sensitized solar cells. Acta Crystallographica Section B: Structural Science, 2012, 68, 137-149. | 1.8 | 26 |
| 57 | Quantitative analysis of hydrogen bonding and atomic thermal motion in the organic non-linear optical material DCNP using X-ray and neutron diffraction. Acta Crystallographica Section B: Structural Science, 2000, 56, 1085-1093. | 1.8 | 25 |
| 58 | Disorder in pentachloronitrobenzene, C6Cl5NO2: a diffuse scattering study. Acta Crystallographica Section B: Structural Science, 2007, 63, 663-673. | 1.8 | 25 |
| 59 | ChemSchematicResolver: A Toolkit to Decode 2D Chemical Diagrams with Labels and R-Groups into Annotated Chemical Named Entities. Journal of Chemical Information and Modeling, 2020, 60, 2059-2072. | 5.4 | 25 |
| 60 | Quantifying Crystallographically Independent Optical Switching Dynamics in Ru SO<sub>2</sub> Photoisomers via Lock-and-Key Crystalline Environment. Journal of Physical Chemistry Letters, 2013, 4, 3221-3226. | 4.6 | 24 |
| 61 | Molecular engineering of cyanine dyes to design a panchromatic response in co-sensitized dye-sensitized solar cells. Molecular Systems Design and Engineering, 2016, 1, 86-98. | 3.4 | 24 |
| 62 | BatteryBERT: A Pretrained Language Model for Battery Database Enhancement. Journal of Chemical Information and Modeling, 2022, 62, 6365-6377. | 5.4 | 24 |
| 63 | Perovskite- and Dye-Sensitized Solar-Cell Device Databases Auto-generated Using ChemDataExtractor. Scientific Data, 2022, 9, . | 5.3 | 24 |
| 64 | Hydride Encapsulation by a Molecular Main-Group-Metal Cluster:Â Single-Crystal Neutron Diffraction Structure of [{Ph(2-C5H4N)N}6HLi8]+. Organometallics, 2004, 23, 4527-4530. | 2.3 | 23 |
| 65 | Solarâ€Powered Nanomechanical Transduction from Crystalline Molecular Rotors. Advanced Materials, 2013, 25, 3324-3328. | 21.0 | 23 |
| 66 | Direct observation ofRâ€¦Rdistances in rare-earth(R)phosphate glasses by magnetic difference neutron diffraction. Physical Review B, 2006, 73, . | 3.2 | 22 |
| 67 | Applications of photocrystallography: a future perspective. Zeitschrift Fur Kristallographie - Crystalline Materials, 2008, 223, 363-369. | 0.8 | 22 |
| 68 | SO<sub>2</sub> Phototriggered Crystalline Nanomechanical Transduction of Aromatic Rotors in Tosylates: Rationalization via Photocrystallography of [Ru(NH<sub>3</sub>)<sub>4</sub>SO<sub>2</sub>X]tosylate<sub>2</sub> (X = pyridine, 3-Cl-pyridine,) Tj ETQq0 0 0 rgBT /Overlock | 3.1 | 22 |
| 69 | Rapid neutron-diffraction data collection for hydrogen-bonding studies: application of the Laue diffractometer (LADI) to the case study zinc (tris)thiourea sulfate. Acta Crystallographica Section A: Foundations and Advances, 2001, 57, 429-434. | 0.3 | 21 |
| 70 | Concerted Mitigation of OÂ·Â·Â·H and C(Ï€)Â·Â·Â·H Interactions Prospects Sixfold Gain in Optical Nonlinearity of Ionic Stilbazolium Derivatives. ACS Applied Materials & Interfaces, 2015, 7, 4693-4698. | 8.0 | 21 |
| 71 | Î·<sup>2</sup>-SO<sub>2</sub> Linkage Photoisomer of an Osmium Coordination Complex. Inorganic Chemistry, 2018, 57, 2673-2677. | 4.0 | 21 |
| 72 | Inverse Design of Materials That Exhibit the Magnetocaloric Effect by Text-Mining of the Scientific Literature and Generative Deep Learning. Chemistry of Materials, 2021, 33, 7217-7231. | 6.7 | 21 |

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| 73 | Auto-generated database of semiconductor band gaps using ChemDataExtractor. Scientific Data, 2022, 9, 193. | 5.3 | 21 |
| 74 | Discovery of SÂ·Â·Â·Câ‰¡N Intramolecular Bonding in a Thiophenylcyanoacrylate-Based Dye: Realizing Charge Transfer Pathways and DyeÂ·Â·Â·TiO<sub>2</sub> Anchoring Characteristics for Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2017, 9, 25952-25961. | 8.0 | 20 |
| 75 | Dye-Anchoring Modes at the DyeÂ·Â·Â·TiO<sub>2</sub> Interface of N3- and N749-Sensitized Solar Cells Revealed by Glancing-Angle Pair Distribution Function Analysis. Journal of Physical Chemistry C, 2020, 124, 11935-11945. | 3.1 | 20 |
| 76 | The structure of the rare-earth phosphate glass (Sm2O3)0.205(P2O5)0.795studied by anomalous dispersion neutron diffraction. Journal of Physics Condensed Matter, 2007, 19, 056002. | 1.8 | 18 |
| 77 | Molecular origins of nonlinear optical activity in zinc tris(thiourea)sulfate revealed by high-resolution x-ray diffraction data andab initiocalculations. Physical Review B, 2013, 88, . | 3.2 | 18 |
| 78 | Nanosecond time-resolved crystallography of photo-induced species: case study and instrument development for high-resolution excited-state single-crystal structure determination. Faraday Discussions, 2003, 122, 119-129. | 3.2 | 17 |
| 79 | Tormat: a program for the automated structural alignment of molecular conformations. Journal of Applied Crystallography, 2008, 41, 955-957. | 4.5 | 17 |
| 80 | Molecular engineering of fluorescein dyes as complementary absorbers in dye co-sensitized solar cells. Molecular Systems Design and Engineering, 2016, 1, 402-415. | 3.4 | 17 |
| 81 | Solid-state photochemistry. CrystEngComm, 2016, 18, 7175-7179. | 2.6 | 17 |
| 82 | Dye Aggregation, Photostructural Reorganization and Multiple Concurrent DyeÂ·Â·Â·TiO<sub>2</sub> Binding Modes in Dye-Sensitized Solar Cell Working Electrodes Containing Benzothiadiazole-Based Dye RK-1. ACS Applied Energy Materials, 2020, 3, 423-430. | 5.1 | 17 |
| 83 | Imaging Dye Aggregation in MK-2, N3, N749, and SQ-2 dyeÂ·Â·Â·TiO<sub>2</sub> Interfaces That Represent Dye-Sensitized Solar Cell Working Electrodes. ACS Applied Energy Materials, 2020, 3, 3230-3241. | 5.1 | 16 |
| 84 | Bayesian Particle Instance Segmentation for Electron Microscopy Image Quantification. Journal of Chemical Information and Modeling, 2021, 61, 1136-1149. | 5.4 | 16 |
| 85 | Predicting Solar-Cell Dyes for Cosensitization. Journal of Physical Chemistry C, 2014, 118, 14082-14090. | 3.1 | 15 |
| 86 | Discovery of Black Dye Crystal Structure Polymorphs: Implications for Dye Conformational Variation in Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2015, 7, 27646-27653. | 8.0 | 15 |
| 87 | Rationalizing the suitability of rhodamines as chromophores in dye-sensitized solar cells: a systematic molecular design study. Molecular Systems Design and Engineering, 2016, 1, 416-435. | 3.4 | 15 |
| 88 | Dyeâ‹¯TiO<sub>2</sub> interfacial structure of dye-sensitised solar cell working electrodes buried under a solution of I<sup>â^'</sup>/I<sub>3</sub><sup>â^'</sup> redox electrolyte. Nanoscale, 2017, 9, 11793-11805. | 5.6 | 15 |
| 89 | Single Model for Organic and Inorganic Chemical Named Entity Recognition in ChemDataExtractor. Journal of Chemical Information and Modeling, 2022, 62, 1207-1213. | 5.4 | 15 |
| 90 | A database of refractive indices and dielectric constants auto-generated using ChemDataExtractor. Scientific Data, 2022, 9, 192. | 5.3 | 15 |

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| 91 | The neutron diffraction anomalous dispersion technique and its application to vitreous Sm2O3Â·4P2O5. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2007, 571, 622-635. | 1.6 | 14 |
| 92 | Coumarin 545: an emission reference dye with a record-low temperature coefficient for ratiometric fluorescence based temperature measurements. Analyst, The, 2015, 140, 1008-1013. | 3.5 | 14 |
| 93 | Material Profiling for Photocrystallography: Relating Single-Crystal Photophysical and Structural Properties of Luminescent Bis-Cyclometalated Iridium-Based Complexes. Crystal Growth and Design, 2013, 13, 1826-1837. | 3.0 | 13 |
| 94 | Dye Nanoaggregate Structures in MK-2, N3, and N749 DyeÂ·Â·Â·TiO<sub>2</sub>Interfaces That Represent Dye-Sensitized Solar Cell Working Electrodes. ACS Applied Energy Materials, 2020, 3, 900-914. | 5.1 | 13 |
| 95 | Auto-generating databases of Yield Strength and Grain Size using ChemDataExtractor. Scientific Data, 2022, 9, . | 5.3 | 13 |
| 96 | Exploiting structure/property relationships in organic non-linear optical materials: developing strategies to realize the potential of TCNQ derivatives. CrystEngComm, 2002, 4, 232-238. | 2.6 | 12 |
| 97 | Multiple Î±-agostic interactions in a metalâ€“methyl complex: the neutron structure of [Mo(NC6H3Pri2-2,6)2Me2]. Chemical Communications, 1998, , 1829-1830. | 4.1 | 11 |
| 98 | Reaction of metallophosphanide anions with MLnX (X = halide) species as a simple route to heterometallic transition metal complexes. Dalton Transactions, 2003, , 1389-1395. | 3.3 | 11 |
| 99 | Molecular rearrangements of diynes coordinated to triosmium carbonyl clusters: reactions of [Os3(Î¼-H)2(CO)10] and [Os3(CO)10(MeCN)2] with 1,4-dipyridylbuta-1,3-diyne. New Journal of Chemistry, 2005, 29, 145-153. | 2.8 | 11 |
| 100 | Temperature insensitive fluorescence intensity in a coumarin monomerâ€“aggregate coupled system. Chemical Communications, 2014, 50, 9329-9332. | 4.1 | 11 |
| 101 | Transforming Benzophenoxazine Laser Dyes into Chromophores for Dyeâ€Sensitized Solar Cells: A Molecular Engineering Approach. Advanced Energy Materials, 2015, 5, 1401728. | 19.5 | 11 |
| 102 | PDFDataExtractor: A Tool for Reading Scientific Text and Interpreting Metadata from the Typeset Literature in the Portable Document Format. Journal of Chemical Information and Modeling, 2022, 62, 1633-1643. | 5.4 | 11 |
| 103 | Solid-State Dilution of Dihydroxybenzophenones with 4,13-Diaza-18-crown-6 for Photocrystallographic Studies. Crystal Growth and Design, 2012, 12, 2277-2287. | 3.0 | 10 |
| 104 | Local Atomic Structure in Photoisomerized Ruthenium Sulfur Dioxide Complexes Revealed by Pair Distribution Function Analysis. Journal of Physical Chemistry C, 2020, 124, 10094-10104. | 3.1 | 10 |
| 105 | Effects of rare-earth co-doping on the local structure of rare-earth phosphate glasses using high and low energy X-ray diffraction. Physical Chemistry Chemical Physics, 2013, 15, 8529. | 2.8 | 9 |
| 106 | How the Shape of Chemical Data Can Enable Data-Driven Materials Discovery. Trends in Chemistry, 2021, 3, 111-119. | 8.5 | 9 |
| 107 | Nanooptomechanical Transduction in a Single Crystal with 100% Photoconversion. Journal of Physical Chemistry C, 2021, 125, 8907-8915. | 3.1 | 9 |
| 108 | ReactionDataExtractor: A Tool for Automated Extraction of Information from Chemical Reaction Schemes. Journal of Chemical Information and Modeling, 2021, 61, 4962-4974. | 5.4 | 9 |

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| 109 | Discovery of High-Performance Organic Non-Linear Optical Molecules by Systematic â€˜Smart Materialâ€™ Design Strategies. Advanced Materials Research, 2010, 123-125, 959-962. | 0.3 | 8 |
| 110 | Rapid build up of nanooptomechanical transduction in single crystals of a ruthenium-based SO<sub>2</sub> linkage photoisomer. Chemical Communications, 2021, 57, 1320-1323. | 4.1 | 8 |
| 111 | Matrix dependence of blue light emission from a novel NH2-functionalized dicyanoquinodimethane derivative. Journal of Physical Organic Chemistry, 2006, 19, 206-213. | 1.9 | 7 |
| 112 | Photoexcited Phenyl Ring Twisting in Quinodimethane Dyes Enhances Photovoltaic Performance in Dye-Sensitized Solar Cells. ACS Applied Energy Materials, 2018, 1, 1127-1139. | 5.1 | 7 |
| 113 | Molecular Origins of the Nonlinear Optical Responses of a Series of Î±-(X-2-Pyridylamino)-o-cresol Chromophores from Concerted X-ray Diffraction, Hyper-Rayleigh Scattering, and Ab Initio Calculations. Journal of Physical Chemistry C, 2019, 123, 665-676. | 3.1 | 7 |
| 114 | Systems Approach of Photoisomerization Metrology for Single-Crystal Optical Actuators: A Case Study of [Ru(SO<sub>2</sub>)(NH<sub>3</sub>)<sub>4</sub>Cl]Cl. Journal of Physical Chemistry C, 2020, 124, 28230-28243. | 3.1 | 7 |
| 115 | Reconstructing Chromatic-Dispersion Relations and Predicting Refractive Indices Using Text Mining and Machine Learning. Journal of Chemical Information and Modeling, 2022, 62, 2670-2684. | 5.4 | 7 |
| 116 | STRUCTURE AND DEVITRIFICATION CHEMISTRY OF RE(PO<SUB>3</SUB>)<SUB>3</SUB> (RE=La, Pr, Nd, Gd, Dy, Y) METAPHOSPHATE GLASSES. Phosphorus Research Bulletin, 2002, 13, 137-146. | 0.6 | 6 |
| 117 | Solid-state effects of monofluorophenyl substitution in dithiadiazolyl radicals: Impact on SÂ·Â·Â·S and SÂ·Â·Â·N interactions and their classification via Hirshfeld surfaces and fingerprint plots. Polyhedron, 2012, 45, 61-70. | 2.2 | 6 |
| 118 | Relating the Structure of Geminal Amido Esters to their Molecular Hyperpolarizability. Journal of Physical Chemistry C, 2016, 120, 29439-29448. | 3.1 | 6 |
| 119 | Topological Analysis of Void Space in Phosphate Frameworks: Assessing Storage Properties for the Environmentally Important Guest Molecules and Ions: CO2, H2O, UO2, PuO2, U, Pu, Sr2+, Cs+, CH4, and H2. ACS Sustainable Chemistry and Engineering, 2016, 4, 4094-4112. | 6.7 | 6 |
| 120 | Molecular engineering of organic and organometallic second-order nonlinear optical materials. , 2019, , 139-176. | | 6 |
| 121 | Predicting Device Parameters for Dye-Sensitized Solar Cells from Electronic Structure Calculations to Reproduce Experiment. ACS Applied Energy Materials, 2020, 3, 4367-4376. | 5.1 | 6 |
| 122 | Electrolyte/Dye/TiO<sub>2</sub> Interfacial Structures of Dye-Sensitized Solar Cells Revealed by In Situ Neutron Reflectometry with Contrast Matching. Langmuir, 2021, 37, 1970-1982. | 3.5 | 6 |
| 123 | Low-energy optical switching of SO<sub>2</sub> linkage isomerisation in single crystals of a ruthenium-based coordination complex. RSC Advances, 2021, 11, 13183-13192. | 3.6 | 6 |
| 124 | Distinction of disorder, classical and quantum vibrational contributions to atomic mean-square amplitudes in dielectric pentachloronitrobenzene. Physical Review B, 2011, 83, . | 3.2 | 5 |
| 125 | L<sub>2,3</sub>-edge x-ray absorption near-edge spectroscopy analysis of photoisomerism in solid rutheniumâ€“sulfur dioxide complexes. Journal of Physics Condensed Matter, 2013, 25, 085505. | 1.8 | 5 |
| 126 | Enumerating Intramolecular Charge Transfer in Conjugated Organic Compounds. Journal of Chemical Information and Modeling, 2020, 60, 6095-6108. | 5.4 | 5 |

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| 127 | `In-situ' charge-density studies of photoinduced phenomena: possibilities for the future?. Acta Crystallographica Section A: Foundations and Advances, 2004, 60, 472-479. | 0.3 | 4 |
| 128 | C-type CeP3O9. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, i138-i139. | 0.2 | 4 |
| 129 | Effects of the [OC<sub>6</sub>F<sub>5</sub>] moiety upon structural geometry: crystal structures of half-sandwich tantalum(V) aryloxide complexes from reaction of Cp*Ta(N<sup> t) Tj ETQq1 1 0.784314 rgBT /Overlock 10 T 5 Section B: Structural Science, 2011, 67, 416-424. | 1.8 | 4 |
| 130 | Assigning Optical Absorption Transitions with Light-Induced Crystal Structures: Case Study of a Single-Crystal Nanooptomechanical Transducer. Journal of Physical Chemistry C, 2021, 125, 15711-15723. | 3.1 | 4 |
| 131 | Multiphase structural models and hyperpolarizability calculations explain second-order nonlinear optical properties of stilbazolium ions. Physical Review Materials, 2020, 4, . | 2.4 | 4 |
| 132 | Bayesian analysis of the evidence for minor components in crystallographic models: an alternative to the Hamilton {cal R} test. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, 324-330. | 0.3 | 3 |
| 133 | Molecular and Supramolecular Origins of Optical Nonlinearity in N-Methylurea. Journal of Physical Chemistry C, 2013, 117, 25669-25676. | 3.1 | 3 |
| 134 | Photochemistry: Solarâ€Powered Nanomechanical Transduction from Crystalline Molecular Rotors (Adv. Mater. 24/2013). Advanced Materials, 2013, 25, 3388-3388. | 21.0 | 3 |
| 135 | X-Ray Diffraction of Photolytically Induced Molecular Species in Single Crystals. , 2008, , 29-61. | | 3 |
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