Jacqueline M Cole

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/3138942/publications.pdf Version: 2024-02-01



#	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 UV–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 UV–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 ₂ 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 Néel 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 [CHâ‹â‹FC] Contacts in Post-Metallocene Polyolefin Catalysts: Modeling Weak Attractive Polymer–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)(η1·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

2

#	Article	lF	CITATIONS
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	Ru–OSO Coordination Photogenerated at 100 K in Tetraammineaqua(sulfur dioxide)ruthenium(II) (±)-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 ₂ -Assisted Photoisomerization of Azo Dyes Using Self-Assembled Monolayers: Case Study on <i>para</i> -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-4′-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 <i>p</i> -Methyl Red Monomeric-to-Pentameric Dye Aggregates on Anatase (101) Titania Surfaces: First-Principles Calculations of Dye/TiO ₂ 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

#	Article	IF	CITATIONS
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€5ensitized 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 host–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 dye···TiO ₂ 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 ₂ ? Case study of dye-to-TiO ₂ adsorption using azo dyes with NO ₂ 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 ₂ Surfaces: Application to Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2015, 7, 16404-16409.	8.0	27

#	Article	IF	CITATIONS
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 ₂ 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 ofR…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 ₂ Phototriggered Crystalline Nanomechanical Transduction of Aromatic Rotors in Tosylates: Rationalization via Photocrystallography of [Ru(NH ₃) ₄ SO ₂ X]tosylate ₂ (X = pyridine, 3-Cl-pyridine,) Tj E		rg <mark>32</mark> /Overloc
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 O···H and C(Ï€)··A·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- ² -SO ₂ 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

#	Article	IF	CITATIONS
73	Auto-generated database of semiconductor band gaps using ChemDataExtractor. Scientific Data, 2022, 9, 193.	5.3	21
74	Discovery of S···C≡N Intramolecular Bonding in a Thiophenylcyanoacrylate-Based Dye: Realizing Charge Transfer Pathways and Dye···TiO ₂ Anchoring Characteristics for Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2017, 9, 25952-25961.	8.0	20
75	Dye-Anchoring Modes at the Dye··À·TiO ₂ 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 and <i>ab initio</i> calculations. 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	<i>Tormat</i> : 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 Dye···TiO ₂ 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	lmaging Dye Aggregation in MK-2, N3, N749, and SQ-2 dye··À·TiO ₂ 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 & amp; 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	Dye⋯TiO ₂ interfacial structure of dye-sensitised solar cell working electrodes buried under a solution of l ^{â^'} /l ₃ ^{â^'} 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

#	Article	IF	CITATIONS
91	The neutron diffraction anomalous dispersion technique and its application to vitreous Sm2O3·4P2O5. 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 Dye··À·TiO ₂ 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 α-agostic interactions in a metal–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(μ-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 monomer–aggregate coupled system. Chemical Communications, 2014, 50, 9329-9332.	4.1	11
101	Transforming Benzophenoxazine Laser Dyes into Chromophores for Dyeâ€ S ensitized 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

#	Article	IF	CITATIONS
109	Discovery of High-Performance Organic Non-Linear Optical Molecules by Systematic â€~Smart Material' 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 ₂ 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 α-(X-2-Pyridylamino)- <i>o</i> -cresol Chromophores from Concerted X-ray Diffraction, Hyper-Rayleigh Scattering, and <i>Ab Initio</i> 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 ₂)(NH ₃) ₄ 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 ₃) ₃ (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 S···S and S···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 ₂ Interfacial Structures of Dye-Sensitized Solar Cells Revealed by <i>In Situ</i> Neutron Reflectometry with Contrast Matching. Langmuir, 2021, 37, 1970-1982.	3.5	6
123	Low-energy optical switching of SO ₂ 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 _{2,3} -edge x-ray absorption near-edge spectroscopy analysis of photoisomerism in solid ruthenium–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

#	Article	IF	CITATIONS
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 ₆ F ₅] moiety upon structural geometry: crystal structures of half-sandwich tantalum(V) aryloxide complexes from reaction of Cp*Ta(N ^{<i>t</i>) Tj ETQq1 1 0.784314}	4 rgBT /Ov 1.8	verlock 10 Tf.
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 <i>N</i> -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
136	Characterizing Interfacial Structures of Dye-Sensitized Solar Cell Working Electrodes. Langmuir, 2022, 38, 871-890.	3.5	3
137	Clustering a database of optically absorbing organic molecules via a hierarchical fingerprint scheme that categorizes similar functional molecular fragments. Journal of Chemical Physics, 2022, 156, 154110.	3.0	3
138	The 4-(3-chloro-4-methylphenyl)-1,2,3,5-dithiadiazol-3-yl radical. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o2514-o2514.	0.2	2
139	Generic Classification Scheme for Second-Order Dipolar Nonlinear Optical Organometallic Complexes That Exhibit Second Harmonic Generation. Journal of Physical Chemistry A, 2019, 123, 702-714.	2.5	2
140	Single-Crystal Optical Actuation Generated by 100% SO2 Linkage Photoisomerization in a Ruthenium-Based Coordination Complex. Journal of Physical Chemistry C, 2021, 125, 20059-20066.	3.1	2
141	Host-guest prospects of neodymium and gadolinium ultraphosphate frameworks for nuclear waste storage: Multi-temperature topological analysis of nanoporous cages in RP5O14. Journal of Solid State Chemistry, 2018, 266, 250-257.	2.9	1
142	Multiple rare-earth ion environments in amorphous(Gd2O3)0.230(P2O5)0.770revealed by gadoliniumK-edge anomalous x-ray scattering. Physical Review Materials, 2018, 2, .	2.4	1
143	Single-Crystal X-Ray Diffraction Studies of Photo-Induced Molecular Species. ChemInform, 2005, 36, no.	0.0	Ο
144	Data-Driven Molecular Engineering of Solar-Powered Windows. Computing in Science and Engineering, 2018, 20, 84-87.	1.2	0

#	Article	IF	CITATIONS
145	Data-driven materials discovery for solar photovoltaics. , 2021, , 129-164.		0
146	Modeling dark- and light-induced crystal structures and single-crystal optical absorption spectra of ruthenium-based complexes that undergo SO2-linkage photoisomerization. Journal of Chemical Physics, 2021, 155, 234111.	3.0	0
147	Structural Capture of η ¹ -OSO to η ² -(OS)O Coordination Isomerism in a New Ruthenium-Based SO ₂ -Linkage Photoisomer That Exhibits Single-Crystal Optical Actuation. Journal of Physical Chemistry C, 2022, 126, 6047-6059.	3.1	0
148	Using Neutrons to See What's Happening Inside a Transparent Solar Cell. Neutron News, 0, , 1-2.	0.2	0
149	Calculating small-angle scattering intensity functions from electron-microscopy images. RSC Advances, 2022, 12, 16656-16662.	3.6	0