

CITATION REPORT

List of articles citing

Crystallography Open Database (COD): an open-access collection of crystal structures and platform for world-wide collaboration

DOI: 10.1093/nar/gkr900

Nucleic Acids Research, 2012, 40, D420-7.

Source: <https://exaly.com/paper-pdf/52772136/citation-report.pdf>

Version: 2024-04-17

This report has been generated based on the citations recorded by exaly.com for the above article. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

#	Paper	IF	Citations
694	Accurate Band Gap Predictions of Semiconductors in the Framework of the Similarity Transformed Equation of Motion Coupled Cluster Theory.		
693	Stability and Compressibility of Cation-Doped High-Entropy Oxide MgCoNiCuZnO5.		
692	Mapping the Pore Architecture of Structured Catalyst Monoliths from Nanometer to Centimeter Scale with Electron and Xray Tomographies.		
691	High-Throughput Screening of MetalOrganic Frameworks for Macroscale Heteroepitaxial Alignment.		
690	Electronic Structure Origins of Surface-Dependent Growth in IIIV Quantum Dots.		
689	Dissolved Carbonate and pH Control the Dissolution of Uranyl Phosphate Minerals in Flow-Through Porous Media.		
688	Advances, Updates, and Analytics for the Computation-Ready Experimental MetalOrganic Framework Database: CoRE MOF 2019.		
687	Use of the Crystallography Open Database as a source of prior knowledge for molecular modelling. 2012 , 68, s21-s21		
686	The Effect of Antimonate, Arsenate, and Phosphate on the Transformation of Ferrihydrite to Goethite, Hematite, Feroxyhyte, and Tripuhyite. 2013 , 61, 11-25		38
685	Kinetic modeling on CO ₂ capture using basic oxygen furnace slag coupled with cold-rolling wastewater in a rotating packed bed. 2013 , 260, 937-46		46
684	Small-molecule 3D structure prediction using open crystallography data. 2013 , 53, 3127-30		15
683	Dielectric, ferroelectric and non-linear optical behavior of crystalline erbium tartrate dihydrate. 2013 , 13, 1928-1932		6
682	Predictive framework for shape-selective separations in three-dimensional zeolites and metal-organic frameworks. 2013 , 29, 5599-608		46
681	Synthesis, Mössbauer Characterization, and Ab Initio Modeling of Iron Oxide Nanoparticles of Medical Interest Functionalized by Dopamine. 2013 , 117, 14295-14302		26
680	MOFomics: Computational pore characterization of metal-organic frameworks. 2013 , 165, 32-39		101
679	In situ X-ray studies of adlayer-induced crystal nucleation at the liquid-liquid interface. 2013 , 110, 6663-8		22
678	New boron nitride structures B4N4: a first-principles random searching application. 2013 , 25, 125504		18

677	Stereochemical statistics in Crystallography Open Database. 2013 , 69, s388-s389	
676	In Situ Dispersive EXAFS in Electrocatalysis: The Investigation of the Local Structure of IrOx in Chronoamperometric Conditions as a Case Study. 2014 , 2014, 1-7	12
675	LACAME 2012. 2014 ,	
674	1. Modern X-ray Diffraction Methods in Mineralogy and Geosciences. 2014 , 1-32	1
673	MolBridge: a program for identifying nonbonded interactions in small molecules and biomolecular structures. 2014 , 47, 1772-1776	14
672	One-click preparation of 3D print files (*.stl, *.wrl) from *.cif (crystallographic information framework) data using Cif2VRML. 2014 , 29, S42-S47	18
671	An intuitive and efficient method for cell voltage prediction of lithium and sodium-ion batteries. 2014 , 5, 5559	33
670	Rectification in tunneling junctions: 2,2'-bipyridyl-terminated n-alkanethiolates. 2014 , 136, 17155-62	78
669	The HighScore suite. 2014 , 29, S13-S18	525
668	Oxidation states of iron as an indicator of the techniques used to burn clays and handcraft archaeological Tupiguarani ceramics by ancient human groups in Minas Gerais, Brazil. 2014 , 224, 121-129	0
667	Synthesis of MnFe ₂ O ₄ nanocrystals by wet-milling under atmospheric conditions. 2014 , 40, 7953-7956	26
666	Slag Formation during Oxygen-Blown Entrained-Flow Gasification of Stem Wood. 2014 , 28, 6941-6952	26
665	Epoxide assisted metal oxide replication (EAMOR): a new technique for metal oxide patterning. 2014 , 4, 36494	3
664	Public Chemical Databases and the Semantic Web. 2014 , 197-217	0
663	An Innovative Pathway towards Nano-Sized Parylene-Based Materials Prepared by Plasma-Based Deposition: Example of Application to the Production of Antimicrobial Materials. 2014 , 11, 489-495	4
662	Structural characteristics and mechanical and thermodynamic properties of nanocrystalline TiO ₂ . 2014 , 114, 9613-44	226
661	Growth and characterization of terbium fumarate heptahydrate single crystals. 2014 , 389, 39-46	9
660	Dielectric, ferroelectric and optical behaviour of terbium hydrogen tartrate trihydrate crystals. 2014 , 49, 4891-4898	8

659	Open Access Resources for Crystallography Education in Interdisciplinary College Courses: Crystallographic Databases and 3D Printed Models. 2014 , 1716, 11	6
658	The Search for Hydrogen Stores on a Large Scale; A Straightforward and Automated Open Database Analysis as a First Sweep for Candidate Materials. 2015 , 5, 617-633	4
657	Enhancing the low frequency THz resonances (2015,	
656	Surface Properties of Clay Minerals. 2015 , 6, 5-31	44
655	Role of N-Donor Sterics on the Coordination Environment and Dimensionality of Uranyl Thiophenedicarboxylate Coordination Polymers. 2015 , 15, 3481-3492	35
654	Iron-containing pigment from an archaeological rupestrian painting of the Planalto Tradition in Minas Gerais, Brazil. 2015 , 232, 29-40	1
653	Accelerated materials property predictions and design using motif-based fingerprints. 2015 , 92,	111
652	Influence of electric discharge activity on bearing lubricating grease degradation. 2015 ,	7
651	Structural and Magnetic Properties of MnxB100 Alloys. 2015 , 51, 1-3	8
650	Computational study of influence of diffuse basis functions on geometry optimization and spectroscopic properties of losartan potassium. 2015 , 137, 1029-38	4
649	Crystal structure refinement with SHELXL. 2015 , 71, 3-8	21059
648	A Molecular Mechanism of Ice Nucleation on Model AgI Surfaces. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 9049-55	3-4 77
647	Limestone Calcination Nearby Equilibrium: Kinetics, CaO Crystal Structure, Sintering and Reactivity. 2015 , 119, 1623-1641	97
646	QUALX2.0: a qualitative phase analysis software using the freely available database POW_COD. 2015 , 48, 598-603	137
645	Growth, characterization and dielectric studies of gadolinium fumarate heptahydrate single crystals. 2015 , 38, 73-81	7
644	Thermal and magnetic properties of lanthanide based metal-organic complex: Neodymium tartrate trihydrate. 2015 , 15, 1251-1255	2
643	Phase transformation of spodumene with hybrid microwave and conventional furnaces. 2015 , 82, 54-60	38
642	Computing stoichiometric molecular composition from crystal structures. 2015 , 48, 85-91	77

641	Computation of electron energy loss spectra by an iterative method. 2015 , 354, 216-219	5
640	3D printed models of small and large molecules, structures and morphologies of crystals, as well as their anisotropic physical properties. 2015 , 50, 432-441	17
639	Discovering Amorphous Indium Phosphide Nanostructures with High-Temperature ab Initio Molecular Dynamics. 2015 , 119, 23238-23249	11
638	Crystallographic education in the 21st century. 2015 , 48, 1964-1975	20
637	Genotoxicity of metal oxide nanomaterials: review of recent data and discussion of possible mechanisms. 2015 , 7, 2154-98	135
636	Materials Screening Through GPU Accelerated Topological Mapping. 2015 , 30, 529-537	3
635	The Effect of Sintering Temperature on Linear and Nonlinear Optical Properties of YAG Nanoceramics. 2015 , 147-164	3
634	Crystallization processes in Ge ₂ Sb ₂ Se ₄ Te glass. 2015 , 61, 207-214	7
633	Linkage isomerism of CO adsorbed on alkali halides. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 2363-70 2.8	1
632	Paramagnetic Manganese in the Atherosclerotic Plaque of Carotid Arteries. 2016 , 2016, 3706280	15
631	Theoretical investigation of electron structure and surface morphology of titanium dioxide anatase nano-particles. 2016 , 1091, 122-136	14
630	Superior Chemical Sensing Performance of Black Phosphorus: Comparison with MoS ₂ and Graphene. 2016 , 28, 7020-8	267
629	Optimization of Synthesis Conditions of Monoclinic Potassium Niobate (KNbO ₃) and its Effect on Morphology. 2016 , 13, 743-752	8
628	Vibrational signatures in the THz spectrum of 1,3-DNB: A first-principles and experimental study. 2016 , 114, 37010	1
627	Strong piezoelectric response in stable TiZnN ₂ , ZrZnN ₂ , and HfZnN ₂ found by ab initio high-throughput approach. 2016 , 120, 225102	6
626	Characterization of Crystalline Structure and Morphology of Ga ₂ O ₃ Thin Film Grown by MOCVD Technique. 2016 , 721, 253-257	1
625	Characterization of structure and thermophysical properties of three ESR slags. 2016 , 143, 012007	
624	A Complete Overhaul of the Electron Energy-Loss Spectroscopy and X-Ray Absorption Spectroscopy Database: eelsdb.eu. 2016 , 22, 717-24	65

623	A polymer dataset for accelerated property prediction and design. <i>Scientific Data</i> , 2016 , 3, 160012	8.2	100
622	Temperature dependent terahertz properties of energetic materials. 2016 ,		1
621	Stable anodes for lithium ion batteries made of self-organized mesoporous silicon. 2016 , 31, 014007		3
620	Structural Changes in RuO ₂ during Electrochemical Hydrogen Evolution. 2016 , 120, 7094-7102		17
619	Biomimetic Random Lasers with Tunable Spatial and Temporal Coherence. 2016 , 4, 1998-2003		12
618	Molecular Simulation of n-Octacosane-Water Mixture in Titania Nanopores at Elevated Temperature and Pressure. 2016 , 120, 24743-24753		12
617	Synthesis of yttrium aluminum garnet nanoparticles in confined environment, and their characterization. 2016 , 511, 82-90		3
616	Comments on "Dental lessons from past to present: ultrastructure and composition of teeth from plesiosaurs, dinosaurs, extinct and recent sharks" by A. L�ke, J. Enax, K. Loza, O. Prymak, P. Gaengler, H.-O. Fabritius, D. Raabe and M. Epple, RSC Adv., 2015, 5, 61612. 2016 , 6, 74384-74388		8
615	Pairs of Ln(III) dopant ions in crystalline solid luminophores: an ab initio computational study. 2016 , 34, 820-827		1
614	On the effect of Sn-doping in hematite anodes for oxygen evolution. 2016 , 214, 345-353		31
613	cif2tube - Algorithm for constructing nanotube and nanoscroll models from crystallographic information files. 2016 , 68, 415-422		2
612	Predicting the Stability of Fullerene Allotropes Throughout the Periodic Table. 2016 , 120, 17035-17045		7
611	A Least-Squares Commutator in the Iterative Subspace Method for Accelerating Self-Consistent Field Convergence. 2016 , 12, 5322-5332		3
610	The optimal one dimensional periodic table: a modified Pettifor chemical scale from data mining. 2016 , 18, 093011		30
609	Composition and fate of mine- and smelter-derived particles in soils of humid subtropical and hot semi-arid areas. 2016 , 563-564, 329-39		25
608	Silicon etch with chromium ions generated by a filtered or non-filtered cathodic arc discharge. 2016 , 17, 20-28		0
607	Toward Structural Correctness: Aquatolide and the Importance of 1D Proton NMR FID Archiving. 2016 , 81, 878-89		31
606	Effects of composition and production route on structure and catalytic activity for ammonia decomposition reaction of ternary Ni-Mo nitride catalysts. 2016 , 41, 3854-3860		30

605	Discovering More Chemical Concepts from 3D Chemical Information Searches of Crystal Structure Databases. 2016 , 93, 550-554		6
604	: an error-correcting CIF parser for the Perl language. 2016 , 49, 292-301		89
603	Metal-boride phase formation on tungsten carbide (WC-Co) during microwave plasma chemical vapor deposition. 2016 , 364, 315-321		17
602	Characterisation of the structure and thermophysical properties of solid electroslag remelting slags. 2016 , 32, 1249-1263		7
601	Vapor and healing treatment for CH ₃ NH ₃ PbI(3-x)Cl(x) films toward large-area perovskite solar cells. 2016 , 8, 6386-92		24
600	Ligand Addition Energies and the Stoichiometry of Colloidal Nanocrystals. 2016 , 10, 1462-74		24
599	Simulations of Ice Nucleation by Kaolinite (001) with Rigid and Flexible Surfaces. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 1726-34	3-4	54
598	AiiDA: automated interactive infrastructure and database for computational science. 2016 , 111, 218-230		275
597	Enhancement of the antimicrobial properties of orthorhombic molybdenum trioxide by thermal induced fracturing of the hydrates. 2016 , 58, 1064-70		16
596	Metakaolin geopolymer characterization and application for ammonium removal from model solutions and landfill leachate. 2016 , 119, 266-276		98
595	Leaching behaviour of slag and fly ash from laterite nickel ore smelting (Niquelândia, Brazil). 2016 , 64, 118-127		22
594	Bond-order reactive force fields for molecular dynamics simulations of crystalline silica. 2016 , 111, 269-276		11
593	High temperature investigation on a nickel transient liquid-phase wafer bonding up to 600 (°C). 2017 , 23, 745-754		5
592	Effect of local structure of Sm ³⁺ in MgAl ₂ O ₄ :Sm ³⁺ phosphors prepared by thermal decomposition of triethanolamine complexes on their luminescence property. 2017 , 701, 1019-1026		34
591	Three-dimensional organic Dirac-line materials due to nonsymmorphic symmetry: A data mining approach. 2017 , 95,		24
590	Geochemical sources, forms and phases of soil contamination in an industrial city. 2017 , 584-585, 505-514		26
589	KSbOSiO ₄ microcrystallites as a source of corrosion of blue-green lead-potassium glass beads of the 19th century. 2017 , 121, 014902		5
588	Tropical river suspended sediment and solute dynamics in storms during an extreme drought. 2017 , 53, 3695-3712		20

- 587 Effect of various types of thermochemical processing of sewage sludges on phosphorus speciation, solubility, and fertilization performance. **2017**, 62, 194-203 43
- 586 Keep it together: restraints in crystallographic refinement of macromolecule-ligand complexes. **2017**, 73, 93-102 18
- 585 Physico-chemical characteristics, biocompatibility, and MRI applicability of novel monodisperse PEG-modified magnetic Fe₃O₄@SiO₂ core-shell nanoparticles. **2017**, 7, 8786-8797 33
- 584 Computer-Assisted Inverse Design of Inorganic Electrides. **2017**, 7, 51
- 583 Characterization of Fe-Mn concentric nodules from Luvisol irrigated by mine water in a semi-arid agricultural area. **2017**, 299, 32-42 17
- 582 Stability of formic acid/pyridine and isonicotinamide/formamide cocrystals by molecular dynamics simulations. **2017**, 136, 1 5
- 581 Samarium doped ceria (SDC) synthesized by a metal triethanolamine complex decomposition method: Characterization and an ionic conductivity study. **2017**, 43, 9823-9830 28
- 580 Experimental and predicted mechanical properties of Cr_{1-x}Al_xN thin films, at high temperatures, incorporating in situ synchrotron radiation X-ray diffraction and computational modelling. **2017**, 7, 22094-22104 14
- 579 Bayesian approach to powder phase identification. **2017**, 50, 776-786 4
- 578 Software Platforms for Electronic/Atomistic/Mesosopic Modeling: Status and Perspectives. **2017**, 6, 92-110 4
- 577 Low-temperature formation and stabilization of rare allotropes of cyclooctasulfur (C₈S₈ and C₈S₈) in the presence of organic carbon at a sulfur-rich glacial site in the Canadian High Arctic. **2017**, 200, 218-231 14
- 576 The pH-dependent leaching behavior of slags from various stages of a copper smelting process: Environmental implications. **2017**, 187, 178-186 42
- 575 Binary Fe-Pd submicron structures fabricated through glancing angle deposition (GLAD) for bioapplications. **2017**, 131, 366-374 9
- 574 Phase evolution, morphology and photodegradation kinetics of hydrothermally synthesized tetragonal sodium niobate. **2017**, 53, 687-699 0
- 573 Accessing Materials Data: Challenges and Directions in the Digital Era. **2017**, 6, 172-186 6
- 572 Kinetic study of the magnesium oxychloride cement cure reaction. **2017**, 52, 7637-7646 16
- 571 Construction of crystal structure prototype database: methods and applications. **2017**, 29, 165901 17
- 570 Surface anisotropy of iron oxide nanoparticles and slabs from first principles: Influence of coatings and ligands as a test of the Heisenberg model. *Journal of Magnetism and Magnetic Materials*, **2017**, 434, 14-22 2.8 3

569	Main features of QUALX2.0 software for qualitative phase analysis. 2017 , 32, S129-S134	8
568	Synthesis and optical characterization of Er-doped bismuth titanate nanoparticles grown by sol-gel hydrothermal method. 2017 , 43, 3623-3630	11
567	Using on site data to study efficiency in industrial granite cutting. 2017 , 166, 1113-1121	5
566	Single-Crystal X-Ray Diffraction. 2017 , 1-28	
565	Reactivity of 12-tungstophosphoric acid and its inhibitor potency toward Na/K-ATPase: A combined P NMR study, ab initio calculations and crystallographic analysis. 2017 , 176, 90-99	10
564	Electron paramagnetic resonance and photoluminescence investigation of europium local structure in oxyfluoride glass ceramics containing SrF ₂ nanocrystals. 2017 , 72, 749-755	16
563	Photothermal Catalyst Engineering: Hydrogenation of Gaseous CO with High Activity and Tailored Selectivity. 2017 , 4, 1700252	59
562	Utilization of precipitated CaCO ₃ from carbon sequestration of industrially emitted CO ₂ in cementless CaO-activated blast-furnace slag binder system. 2017 , 166, 649-659	16
561	Band gap engineering of niobate composites through incorporation of Ni ²⁺ metal ions and its property evaluation. 2017 , 53, 701-711	0
560	Data Mining for Three-Dimensional Organic Dirac Materials: Focus on Space Group 19. 2017 , 7, 7298	19
559	Synthesis of zinc oxide powders in plasma-solution systems. 2017 , 51, 65-69	13
558	Effects of grain size, mineralogy, and acid-extractable grain coatings on the distribution of the fallout radionuclides ⁷ Be, ¹⁰ Be, ¹³⁷ Cs, and ²¹⁰ Pb in river sediment. 2017 , 197, 71-86	29
557	Chlorhexidine digluconate on chitosan-magnetic iron oxide nanoparticles modified electrode: Electroanalysis and mechanistic insights by computational simulations. 2017 , 240, 417-425	15
556	Use of metal/metal oxide spherical cluster and hydroxyl metal coordination complex for descriptor calculation in development of nanoparticle cytotoxicity classification model. 2017 , 28, 875-888	6
555	A posteriori metadata from automated provenance tracking: integration of AiiDA and TCOD. 2017 , 9, 56	15
554	Effect of Calcium Carbonate Fineness on Calcium Sulfoaluminate-Belite Cement. 2017 , 10,	35
553	. 2017 ,	1
552	FT-IR and Raman Spectroscopies, Polymorphism Applications. 2017 , 750-761	4

551	Effect of Ni-Content on the Transformation Temperatures in NiTi-20 at. % Zr High Temperature Shape Memory Alloys. 2017 , 7, 511	17
550	Organic materials database: An open-access online database for data mining. 2017 , 12, e0171501	34
549	AceDRG: a stereochemical description generator for ligands. 2017 , 73, 112-122	144
548	Strategies for carbohydrate model building, refinement and validation. 2017 , 73, 171-186	34
547	X-ray Crystallography of Small Molecules: Theory and Workflow ?. 2017 , 624-639	1
546	Potassium gadolinium tungstate nanocrystals doped with holmium ions as candidates for optical imaging. 2018 , 446, 139-144	7
545	In Situ Synchrotron Radiation X-ray Diffraction Study on Phase and Oxide Growth during a High Temperature Cycle of a NiTi-20 at.% Zr High Temperature Shape Memory Alloy. 2018 , 4, 174-185	12
544	X-ray reflectivity from curved liquid interfaces. 2018 , 25, 432-438	3
543	Mineralogical investigations using XRD, XRF, and Raman spectroscopy in a combined approach. 2018 , 49, 1023-1030	15
542	Comparing results of X-ray diffraction, μ -Raman spectroscopy and neutron diffraction when identifying chemical phases in seized nuclear material, during a comparative nuclear forensics exercise. 2018 , 315, 395-408	5
541	Fast One-Pot Photosynthesis of Plasmonic Protein-Coated Silver/Silver Bromide Nanoparticles with Efficient Photocatalytic Performance. 2018 , 28, 2056-2062	5
540	Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds. 2018 , 13, 246-252	874
539	In silico study toward the identification of new and safe potential inhibitors of photosynthetic electron transport. 2018 , 153, 175-180	0
538	From Cubic Palladium to Concave Core-Shell Platinum Palladium Nanoparticles: Evolution of the Structure and Their Electrochemical Properties. 2018 , 165, H67-H77	3
537	Characterization and pH-dependent environmental stability of arsenic trioxide-containing copper smelter flue dust. 2018 , 209, 71-80	33
536	Uranium speciation in acid waste-weathered sediments: The role of aging and phosphate amendments. 2018 , 89, 109-120	12
535	The hitchhiker's guide to the chemical-biological galaxy. 2018 , 23, 565-574	21
534	Phase Transformation Mechanism of Li-Ion Storage in Iron(III) Hydroxide Phosphates. 2018 , 122, 1930-1938	5

533	Size-dependent disproportionation (in ~ 20 nm regime) and hybrid Bond Valence derived interatomic potentials for BaTaO ₂ N. 2018 , 8, 1379-1388	2
532	Transformation of arsenic-rich copper smelter flue dust in contrasting soils: A 2-year field experiment. 2018 , 237, 83-92	13
531	Big Data in Drug Discovery. 2018 , 57, 277-356	25
530	Phasing via pure crystallographic least squares: an unexpected feature. 2018 , 74, 123-130	
529	Nonresonant valence-to-core x-ray emission spectroscopy of niobium. 2018 , 97,	8
528	Charge transport in organic molecular semiconductors from first principles: The bandlike hole mobility in a naphthalene crystal. 2018 , 97,	44
527	Tailoring Surface Frustrated Lewis Pairs of InO (OH) for Gas-Phase Heterogeneous Photocatalytic Reduction of CO by Isomorphous Substitution of In with Bi. 2018 , 5, 1700732	60
526	Oral bioaccessibility of inorganic contaminants in waste dusts generated by laterite Ni ore smelting. 2018 , 40, 1699-1712	6
525	Catalytic dehydrogenation of ethanol into acetaldehyde and isobutanol using mono- and multicomponent copper catalysts. 2018 , 21, 194-209	24
524	Experimental and theoretical study to explain the morphology of CaMoO ₄ crystals. 2018 , 114, 141-152	31
523	Copper isotopic record in soils and tree rings near a copper smelter, Copperbelt, Zambia. 2018 , 621, 9-17	18
522	Synthesis of CdO Ultradisperse Powders Using Atmospheric Pressure Glow Discharge in Contact With Solution and the Investigation of Intermediate Products. 2018 , 38, 107-121	7
521	Operando SXR D of E-ALD deposited sulphides ultra-thin films: Crystallite strain and size. 2018 , 432, 53-59	5
520	A high-throughput data analysis and materials discovery tool for strongly correlated materials. 2018 , 4,	12
519	Preparing 3D Print Files for Nano-Tech/Science Education from Entries of Large Open-Access Crystallographic Databases at Dedicated Websites. 2018 ,	
518	An open-source software ecosystem for the interactive exploration of ultrafast electron scattering data. 2018 , 4, 11	6
517	Two-step magnetic transition in hybrid organic-inorganic materials of the (m-xylylenediamine)MeSO ₄ (Me = Mn, Fe, Co, Ni) type. 2018 , 42, 18225-18235	1
516	A high-performance and flexible chemical structure & data search engine built on CouchDB & ElasticSearch. 2018 , 31, 341-349	3

515	Open-Science Platform for Computational Materials Science: AiiDA and the Materials Cloud. 2018 , 1-24	
514	Crystallography Open Database (COD). 2018 , 1-19	1
513	Polymer morphology and interfacial charge transfer dominate over energy-dependent scattering in organic-inorganic thermoelectrics. 2018 , 9, 5347	41
512	Ni- and Sb-Doped SnO ₂ Electrocatalysts with High Current Efficiency for Ozone Production via Electrodeposited Nanostructures. 2018 , 165, E833-E840	8
511	The use of limestone to replace physical filler of quartz powder in UHPFRC. 2018 , 94, 238-247	32
510	New developments in low clinker cement paste mineralogy. 2018 , 166, 94-101	8
509	Refining the macromolecular model - achieving the best agreement with the data from X-ray diffraction experiment. 2018 , 24, 236-262	24
508	Machine Learning and Big-Data in Computational Chemistry. 2018 , 1-24	3
507	NanoCrystal: A Web-Based Crystallographic Tool for the Construction of Nanoparticles Based on Their Crystal Habit. 2018 , 58, 2380-2386	11
506	Effects of point defects on the mechanical response of LaRu ₂ P ₂ . 2018 , 160, 224-234	4
505	Encyclopedia of Big Data Technologies. 2018 , 1-8	1
504	Influence of Salinity and Pb on the Precipitation of Zn in a Model System. <i>Minerals (Basel, Switzerland)</i> , 2018 , 8, 43	2.4 7
503	Learning from Correlations Based on Local Structure: Rare-Earth Nickelates Revisited. 2018 , 58, 2491-2501	6
502	Revisiting models of Cd, Cu, Pb and Zn adsorption onto Fe(III) oxides. 2018 , 493, 189-198	31
501	Cluster structures influenced by interaction with a surface. 2018 , 20, 15661-15670	5
500	Multisite formation in gadolinium doped SrF ₂ nanoparticles. 2018 , 762, 500-507	3
499	Stabilization of molten salt materials using metal chlorides for solar thermal storage. 2018 , 8, 8190	9
498	Growth of trigonal gadolinium fluoride in a glass-ceramic for scintillation and optical applications. 2018 , 38, 4739-4748	4

497	Restricted Open-Shell Configuration Interaction Singles Study on M- and L-edge X-ray Absorption Spectroscopy of Solid Chemical Systems. 2018 , 14, 4320-4334		11
496	Existence of a Preferred Orientation for the Methoxy Group on an Extended Aromatic System.. 2018 , 3, 6750-6755		2
495	Iron Phase Stabilized at Room Temperature by Thermally Processed Graphene Oxide. 2018 , 140, 9051-9055		14
494	Towards Generalized Noise-Level Dependent Crystallographic Symmetry Classifications of More or Less Periodic Crystal Patterns. 2018 , 10, 133		7
493	OChemDb: the free online Open Chemistry Database portal for searching and analysing crystal structure information. 2018 , 51, 1229-1236		7
492	Phase Diagrams of TIP4P/2005, SPC/E, and TIP5P Water at High Pressure. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 7718-7725	3-4	22
491	Free-energy analysis of physisorption on solid-liquid interface with the solution theory in the energy representation. 2018 , 149, 014504		4
490	Evolution of Photoluminescence, Raman, and Structure of CHNHPbI Perovskite Microwires Under Humidity Exposure. 2018 , 13, 79		21
489	Mechanical alloying and theoretical studies of MnAl(C) magnets. <i>Journal of Magnetism and Magnetic Materials</i> , 2018 , 462, 96-104	2.8	14
488	Structural biology data archiving - where we are and what lies ahead. 2018 , 592, 2153-2167		8
487	Using SMILES strings for the description of chemical connectivity in the Crystallography Open Database. 2018 , 10, 23		60
486	Natural speciation of nickel at the micrometer scale in serpentine (ultramafic) topsoils using microfocused X-ray fluorescence, diffraction, and absorption. 2018 , 19, 14		10
485	Synthesis of NaAlH ₄ /Al composites and their applications in hydrogen storage. 2018 , 43, 17309-17317		17
484	Genotoxicity induced by metal oxide nanoparticles: a weight of evidence study and effect of particle surface and electronic properties. 2018 , 12, 1113-1129		17
483	Evaluation of metal type in MIL-100 structure to synthesize a selective adsorbent for the basic N-compounds removal from liquid fuels. 2019 , 274, 54-60		7
482	High-throughput computational screening of layered and two-dimensional materials. 2019 , 9, e1385		26
481	Toricelli: A software to determine atomic spatial distributions from normal incidence x-ray standing wave data. 2019 , 235, 502-513		10
480	Recent advances and applications of machine learning in solid-state materials science. 2019 , 5,		631

479	Combined XRF, XRD, SEM-EDS, and Raman Analyses on Serpentinized Harzburgite (Nickel Laterite Mine, New Caledonia): Implications for Exploration and Geometallurgy. 2019 , 3, 2237-2249	7
478	Fast, efficient fragment-based coordinate generation for Open Babel. 2019 , 11, 49	12
477	Mineralogical Diversity of Ca ₂ SiO ₄ -Bearing Combustion Metamorphic Rocks in the Hatrurim Basin: Implications for Storage and Partitioning of Elements in Oil Shale Clinkering. <i>Minerals (Basel, Switzerland)</i> , 2019 , 9, 465	2.4 15
476	Data-Driven Systematic Search of Promising Photocatalysts for Water Splitting under Visible Light. 2019 , 10, 5211-5218	17
475	Accelerated Discovery of Efficient Solar-cell Materials using Quantum and Machine-learning Methods. 2019 , 31,	48
474	Structural and Photoelectric Properties of Epitaxially Grown Vanadium Dioxide Thin Films on c-Plane Sapphire and Titanium Dioxide. 2019 , 9, 9362	8
473	Multi-response optimization of MIL-101 synthesis for selectively adsorbing N-compounds from fuels. 2019 , 16, 1442-1454	1
472	Characterization of a system that combines energy dispersive X-ray diffraction with X-ray fluorescence and its potential applications in archeometry. 2019 , 126, 044901	4
471	Two-Dimensional van der Waals Materials with Aligned In-Plane Polarization and Large Piezoelectric Effect for Self-Powered Piezoelectric Sensors. 2019 , 19, 5410-5416	74
470	Accurate Band Gap Predictions of Semiconductors in the Framework of the Similarity Transformed Equation of Motion Coupled Cluster Theory. 2019 , 58, 9303-9315	29
469	Effect of testing conditions on the dry sliding behavior of a Cu-Based refractory composite material. 2019 , 140, 105850	12
468	Stability and Compressibility of Cation-Doped High-Entropy Oxide MgCoNiCuZnO ₅ . 2019 , 123, 17735-17744	23
467	Accelerated Discovery of Two-Dimensional Optoelectronic Octahedral Oxyhalides via High-Throughput Calculations and Machine Learning. 2019 , 10, 6734-6740	20
466	Medium-scale Plant Experiment of Sewage Sludge-based Phosphorus Fertilizers from Large-scale Thermal Processing. 2019 , 50, 2469-2481	5
465	Why β -Alumina Is an Effective Ice Nucleus. 2019 , 123, 26424-26431	3
464	Materials Databases: The Need for Open, Interoperable Databases with Standardized Data and Rich Metadata. 2019 , 2, 1900131	11
463	Data-Driven Materials Science: Status, Challenges, and Perspectives. 2019 , 6, 1900808	162
462	Mutations in the PKM2 exon-10 region are associated with reduced allostery and increased nuclear translocation. 2019 , 2, 105	7

461	The Regulatory Role of Long Noncoding RNAs in Different Brain Cell Types Involved in Ischemic Stroke. 2019 , 12, 61	18
460	Crystallography Open Database: History, Development, and Perspectives. 2019 , 1-39	1
459	Determination of Primary Mineral Content and Calcium Sources in Forest Soils using Electron Probe Microanalysis Mapping and Cluster Analysis. 2019 , 83, 1830-1841	2
458	From Topological Descriptors to Expert Systems: A Route to Predictable Materials. 2019 , 107-147	2
457	Mining and mineral processing. 2019 , 793-803	1
456	Crystallographic databases and powder diffraction. 2019 , 304-324	4
455	Structural and Electrical Studies for Birnessite-Type Materials Synthesized by Solid-State Reactions. 2019 , 9,	9
454	Theory and simulations of critical temperatures in CrI ₃ and other 2D materials: easy-axis magnetic order and easy-plane Kosterlitz-Thouless transitions. 2019 , 9, 1142-1150	23
453	Identification Schemes for Metal-Organic Frameworks To Enable Rapid Search and Cheminformatics Analysis. 2019 , 19, 6682-6697	59
452	Thermochemical characterization of Zr/Fe ₂ O ₃ pyrotechnic mixture under natural aging conditions. 2019 , 126, 105113	5
451	High-Temperature Tribo-Oxidative Wear of a Cu-Based Metal-Matrix Composite Dry Sliding Against Heat-Treated Steel. 2019 , 67, 1	7
450	Andosolization of ferrallitic soils in the Bambouto Mountains, West Cameroon. 2019 , 340, 81-93	9
449	Comparison of physical and mechanical properties of civil construction plaster and recycled waste gypsum from Sã Paulo, Brazil. 2019 , 22, 504-512	14
448	1.86 Ga key paleomagnetic pole from the Murmansk craton intrusions âEastern Murman Sill Province, NE Fennoscandia: Multidisciplinary approach and paleotectonic applications. 2019 , 324, 126-145	11
447	Oral bioaccessibility of metal(loid)s in dust materials from mining areas of northern Namibia. 2019 , 124, 205-215	31
446	Structure and catalytic activity of ultrasmall Rh, Pd and (Rh + Pd) nanoparticles obtained by mediated electrosynthesis. 2019 , 43, 3931-3945	10
445	Correlative study of lattice imperfections in long-range ordered, nano-scale domains in a Fe-Co-Mo alloy. 2019 , 204, 91-100	3
444	Nanostructured Cobalt-Containing Carbon Supports for New Platinum Catalysts. 2019 , 55, 438-448	0

443	Evaluation of heavy metals background in the Adriatic Sea sediments of Abruzzo region, Italy. 2019 , 684, 445-457		8
442	Influence of polymeric precursors on the viability of human cells of yttrium aluminum borates nanoparticles doped with ytterbium ions. 2019 , 488, 874-886		1
441	Sliding wear of a self-mated thermally sprayed chromium oxide coating in a simulated PWR water environment. 2019 , 426-427, 1466-1473		5
440	Rapid Structure Determination of Molecular Solids Using Chemical Shifts Directed by Unambiguous Prior Constraints. 2019 , 141, 16624-16634		26
439	Rapid dry exfoliation method for tuneable production of molybdenum disulphide quantum dots and large micron-dimension sheets. 2019 , 11, 11626-11633		3
438	Neural network based classification of crystal symmetries from x-ray diffraction patterns. 2019 , 99,		29
437	2DMatPedia, an open computational database of two-dimensional materials from top-down and bottom-up approaches. <i>Scientific Data</i> , 2019 , 6, 86	8.2	92
436	Machine Learning for Computational Heterogeneous Catalysis. 2019 , 11, 3581-3601		127
435	Using porous iron composite (PIC) material to immobilize rhenium as an analogue for technetium. 2019 , 128, 379-389		4
434	Computational Discovery and Design of MXenes for Energy Applications: Status, Successes, and Opportunities. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 24885-24905	9.5	65
433	High-volume use of limestone in ultra-high performance fiber-reinforced concrete for reducing cement content and autogenous shrinkage. 2019 , 213, 292-305		31
432	Encrustations on ureteral stents from patients without urinary tract infection reveal distinct urotypes and a low bacterial load. 2019 , 7, 60		12
431	Stereochemistry of polypeptoid chain configurations. 2019 , 110, e23266		8
430	Prediction of Synthesis of 2D Metal Carbides and Nitrides (MXenes) and Their Precursors with Positive and Unlabeled Machine Learning. 2019 , 13, 3031-3041		95
429	Asymmetric mullite membranes manufactured by phase-inversion tape casting from polymethylsiloxane and aluminum diacetate. 2019 , 581, 421-429		8
428	Managing uncertainty in data-derived densities to accelerate density functional theory. 2019 , 2, 034001		7
427	Thermal Path Reconstruction for Reinforced Concrete Under Fire. 2019 , 55, 1451-1475		4
426	Molecular Driving Forces in Peptide Adsorption to Metal Oxide Surfaces. 2019 , 35, 5911-5920		18

425	Towards rechargeable zinc-air batteries with aqueous chloride electrolytes. 2019 , 7, 11387-11399	34
424	The physicochemical investigation of hydrothermally reduced textile waste and application within carbon-based electrodes.. 2019 , 9, 11239-11252	8
423	The Effect of Surface Reconstruction on the Oxygen Reduction Reaction Properties of LaMnO ₃ . 2019 , 123, 11621-11627	13
422	Pressure-Induced Phase Transitions of Natural Brookite. 2019 , 3, 844-853	4
421	A descriptor of "material genes"—Effective atomic size in structural unit of ionic crystals. 2019 , 62, 849-855	4
420	Laboratory EXAFS determined structure of the stable complexes in the ternary Ni(ii)-EDTA-CN system. 2019 , 21, 9239-9245	4
419	Indium Tin Oxide Film Characteristics for Cathodic Stripping Voltammetry. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 16991-17000	9.5 5
418	The Effect of Elevated Curing Temperatures on High Ye'elite Calcium Sulfoaluminate Cement Mortars. 2019 , 12,	15
417	Friedman method kinetic analysis of CaO-based sorbent for high-temperature thermochemical energy storage. 2019 , 200, 236-247	21
416	Encyclopedia of Big Data Technologies. 2019 , 366-366	
415	LaMgAl ₁₁ O ₁₉ synthesis using non-hydrolytic sol-gel methods. 2019 , 45, 11233-11240	4
414	Phase transformation and structure evolution of a Ti-45Al-7.5Nb alloy processed by high-pressure torsion. 2019 , 787, 1149-1157	7
413	Two-dimensional nonlinear optical materials predicted by network visualization. 2019 , 4, 586-596	3
412	Highly-transparent and conductive CuI films obtained by a redirected low-cost and electroless two-step route: Chemical solution deposition of Cu ₂ S and subsequent iodination. 2019 , 95, 59-67	12
411	Palaeointensities of Oligocene and Miocene volcanic sections from Ethiopia: field behaviour during the Cainozoic. 2019 , 216, 1482-1494	4
410	The Powder Diffraction File: a quality materials characterization database. 2019 , 34, 352-360	321
409	Direct Growth on Si(100) of Isolated Octahedral Mil-101(Fe) Crystals for the Separation of Aromatic Vapors. 2019 , 123, 28836-28845	8
408	Molecular Geometry Prediction using a Deep Generative Graph Neural Network. 2019 , 9, 20381	24

407	Decoding crystallography from high-resolution electron imaging and diffraction datasets with deep learning. 2019 , 5, eaaw1949		43
406	Reducing the crystallite and particle size of SrFe ₂ O ₁₉ with PVA by high energy ball milling. 2019 , 771, 464-470		8
405	First principles study of structural properties and electric field gradients in kaolinite. 2019 , 169, 67-73		14
404	Heterogeneous growth of continuous ZIF-8 films on low-temperature amorphous silicon. 2019 , 473, 182-189		5
403	Electronic mobility and crystal structures of 2,5-dimethylanilinium triiodide and tin-based organic-inorganic hybrid compounds. 2019 , 270, 593-600		5
402	Influence of biofilms on morbidity associated with short-term indwelling ureteral stents: a prospective observational study. 2019 , 37, 1703-1711		6
401	Synthesis of MoO ₃ by glow discharge in contact with water. 2019 , 21, 025505		8
400	Determination of polaronic conductivity in disordered double perovskite La ₂ CrMnO ₆ . 2019 , 42, 136-146		5
399	The formation of a homogeneous alumina coating on a Ni-based superalloy from a layer stack deposited by cathodic arc evaporation. <i>Surface and Coatings Technology</i> , 2019 , 360, 329-334	4-4	1
398	Effect of particle size of nanosilica on microstructure of C-S-H and its impact on mechanical strength. 2019 , 97, 312-321		36
397	Atomically Thin 2D Transition Metal Oxides: Structural Reconstruction, Interaction with Substrates, and Potential Applications. 2019 , 6, 1801160		63
396	Topology-based crystal structure generator. 2019 , 236, 1-7		41
395	Phosphoric acid-modified magnesium oxychloride: Study of water stability, kinetics, and pair distribution function. 2019 , 102, 3728-3737		5
394	Technology in the Service of Pedagogy: Teaching with Chemistry Databases. 2019 , 59, 572-582		5
393	The use of rice husk ash as reactive filler in ultra-high performance concrete. 2019 , 115, 389-400		104
392	Extraction of Silica from Sugarcane Bagasse, Cassava Periderm and Maize Stalk: Proximate Analysis and Physico-Chemical Properties of Wastes. 2019 , 10, 617-629		22
391	Autonomous Discovery in the Chemical Sciences Part II: Outlook. 2020 , 59, 23414-23436		62
390	Autonome Entdeckung in den chemischen Wissenschaften, Teil II: Ausblick. 2020 , 132, 23620-23643		0

389	Anisotropic magnetoresistance behaviors in the layered ferromagnetic Cr ₂ Ge ₂ Te ₆ . 2020 , 53, 025101		5
388	Exploring the Reliability of DFT Calculations of the Infrared and Terahertz Spectra of Sodium Peroxodisulfate. 2020 , 41, 382-413		3
387	High-throughput computational screening for solid-state Li-ion conductors. <i>Energy and Environmental Science</i> , 2020 , 13, 928-948	35.4	42
386	The role of ferrite-cementite interface in formation of hierarchical film on carbon steel in CO ₂ -saturated brine. 2020 , 509, 145107		4
385	Atmospheric corrosion of boron doped iron phosphate glass studied by Raman spectroscopy. <i>Journal of Non-Crystalline Solids</i> , 2020 , 530, 119748	3.9	6
384	Characterization of the precipitation behavior and resulting mechanical properties of copper-alloyed ferritic steel. 2020 , 772, 138807		9
383	Vanadium-rich slags from the historical processing of Zn&Pb&V ores at Berg Aukas (Namibia): Mineralogy and environmental stability. 2020 , 114, 104473		6
382	Crystallographic prediction from diffraction and chemistry data for higher throughput classification using machine learning. 2020 , 173, 109409		18
381	Factor Analysis of XRF and XRPD Data on the Example of the Rocks of the Kontozero Carbonatite Complex (NW Russia). Part II: Geological Interpretation. 2020 , 10, 873		2
380	Factor Analysis of XRF and XRPD Data on the Example of the Rocks of the Kontozero Carbonatite Complex (NW Russia). Part I: Algorithm. 2020 , 10, 874		2
379	Electrochemical crystallization for phosphate recovery from an electronic industry wastewater effluent using sacrificial iron anodes. 2020 , 276, 124234		8
378	Machine learning for halide perovskite materials. 2020 , 78, 105380		27
377	Computation of NMR Shielding Constants for Solids Using an Embedded Cluster Approach with DFT, Double-Hybrid DFT, and MP2. 2020 , 16, 6950-6967		12
376	Quantum anomalous Hall effect in two-dimensional magnetic insulator heterojunctions. 2020 , 6,		11
375	High-performance light-driven heterogeneous CO catalysis with near-unity selectivity on metal phosphides. 2020 , 11, 5149		25
374	Formation of secondary mineral coatings and the persistence of reduced metal-bearing phases in soils developing on historic coal mine spoil. 2020 , 121, 104711		4
373	Site-specific dynamic nuclear polarization in a Gd(III)-labeled protein. 2020 , 22, 25455-25466		7
372	Theoretical approach for calculation of dielectric functions of plasmonic nanoparticles of noble metals, magnesium and their alloys. 2020 , 109, 110264		2

371	Determining dimensionalities and multiplicities of crystal nets. 2020 , 6,		2
370	Destabilized Calcium Hydride as a Promising High-Temperature Thermal Battery. 2020 , 124, 17512-17519		3
369	Thermochemical energy storage performance of zinc destabilized calcium hydride at high-temperatures. 2020 , 22, 25780-25788		2
368	Origin of Magnetotransport Properties in APCVD Deposited Tin Oxide Thin Films. 2020 , 13,		1
367	High-Performance, Scalable, and Low-Cost Copper Hydroxyapatite for Photothermal CO ₂ Reduction. 2020 , 10, 13668-13681		19
366	Kinetics and Mechanism of Turanite Reduction by Hydrogen. 2020 , 124, 18356-18365		1
365	Vanadium in slags from smelting of African Pb-Zn vanadate ores: Mineralogy, extractability and potential recovery. 2020 , 218, 106631		7
364	Removal of ammonium from wastewater with geopolymer sorbents fabricated via additive manufacturing. 2020 , 195, 109006		15
363	An artificial intelligence-aided virtual screening recipe for two-dimensional materials discovery. 2020 , 6,		14
362	Stable Silicene Wrapped by Graphene in Air. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 40620-40628		3
361	Nonempirical Definition of the Mendeleev Numbers: Organizing the Chemical Space. 2020 , 124, 23867-23878		7
360	New Insights into Osteointegration and Delamination from a Multidisciplinary Investigation of a Failed Hydroxyapatite-Coated Hip Joint Replacement. 2020 , 13,		1
359	Controlled synthesis and characterization of NaYF ₃ :Yb/Er upconverting nanoparticles produced by laser ablation in liquid. 2020 , 153, 064701		1
358	3-D Inorganic Crystal Structure Generation and Property Prediction via Representation Learning. 2020 , 60, 4518-4535		16
357	AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance. <i>Scientific Data</i> , 2020 , 7, 300	8.2	49
356	Materials Cloud, a platform for open computational science. <i>Scientific Data</i> , 2020 , 7, 299	8.2	70
355	Insight into the partial replacement of cement by ferronickel slags from New Caledonia. 2020 , 1-19		4
354	Synthesis of copper oxide thin films by electrolysis method based on Porous Silicon for Solar Cell Applications. 2020 , 757, 012051		0

353	A Combined Pyro- and Hydrometallurgical Approach to Recycle Pyrolyzed Lithium-Ion Battery Black Mass Part 1: Production of Lithium Concentrates in an Electric Arc Furnace. 2020 , 10, 1069		14
352	Identification of strongly interacting organic semimetals. 2020 , 102,		2
351	Thermodynamics and Structural Properties of Ti ₃ SiC ₂ in Liquid Lead Coolant. <i>Journal of Physics: Conference Series</i> , 2020 , 1493, 012026	0.3	0
350	An investigation into the temperature phase transitions of synthesized lithium titanate materials doped with Al, Co, Ni and Mg by in situ powder X-ray diffraction. 2020 , 35, 233-246		
349	Effects of Inorganic Ions on Ice Nucleation by the Al Surface of Kaolinite Immersed in Water. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 4605-4618	3-4	11
348	Microstructural and thermal response evolution of metallic form-stable phase change materials produced from ball-milled powders. 2020 , 142, 85-96		6
347	Tracing iron ore tailings in the marine environment: An investigation of the Fundø dam failure. 2020 , 257, 127184		4
346	On cobalt ferrite production by sol-gel from orange fruit residue by three related procedures and its application in oil removal. 2020 , 265, 121712		6
345	Emergence of quasi-two-dimensional electron gas at the interface of LaAlO ₃ /Sr ₂ AlNbO ₆ (001) heterostructures. 2020 , 127, 225303		
344	Multiscale and Multispectral Characterization of Mineralogy with the ExoMars 2022 Rover Remote Sensing Payload. 2020 , 7, e2019EA000692		1
343	Direct Correlation of Charge Carrier Transport to Local Crystal Quality in Lead Halide Perovskites. 2020 , 20, 5050-5056		7
342	High-throughput density functional perturbation theory and machine learning predictions of infrared, piezoelectric, and dielectric responses. 2020 , 6,		22
341	Synthesis and characterization of a novel microporous lanthanide based metal-organic framework (MOF) using naphthalenedicarboxylate acid. 2020 , 9, 7409-7417		18
340	Recombination luminescence of X-ray induced paramagnetic defects in BaY ₂ F ₈ . 2020 , 223, 117216		
339	Magnetic and superconducting phase diagrams and transition temperatures predicted using text mining and machine learning. 2020 , 6,		24
338	The mining of materials with similar electronic properties from the Crystallographic Open Database (COD). 2020 , 7, 035903		1
337	Automated mineralogy for quantification and partitioning of metal(loid)s in particulates from mining/smelting-polluted soils. 2020 , 266, 115118		8
336	Phonon Spectra of Strongly Luminescent Nonstoichiometric Ag ₂ Te, Cu ₂ Te, and Hg ₂ Te Nanocrystals of Small Size. 2020 , 124, 15511-15522		5

335	Slag dusts from Kabwe (Zambia): Contaminant mineralogy and oral bioaccessibility. 2020 , 260, 127642		17
334	A high-power and long-life aqueous rechargeable Zn-ion battery based on hierarchically porous sodium vanadate. 2020 , 56, 9174-9177		9
333	3DStructGen: an interactive web-based 3D structure generation for non-periodic molecule and crystal. 2020 , 12, 7		2
332	A-site cation influences on performance, structure and conductivity of a lanthanide-based perovskite electrode for symmetrical solid oxide fuel cells. 2020 , 450, 227723		2
331	Porous hydrated ammonium vanadate as a novel cathode for aqueous rechargeable Zn-ion batteries. 2020 , 56, 3785-3788		15
330	Spatially Resolved Organomineral Interactions across a Permafrost Chronosequence. 2020 , 54, 2951-2960		9
329	Impact of zero valent iron aging on reductive removal of technetium-99. 2020 , 8, 103767		6
328	Screening Promising Thermoelectric Materials in Binary Chalcogenides through High-Throughput Computations. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 11852-11864	9.5	22
327	Discovering new perovskites with artificial intelligence. 2020 , 285, 121253		7
326	Machine learning: Accelerating materials development for energy storage and conversion. 2020 , 2, 553-576		86
325	The influence of the recycling stress history on LDPE waste pyrolysis. 2020 , 86, 106460		8
324	BOKEI: Bayesian optimization using knowledge of correlated torsions and expected improvement for conformer generation. 2020 , 22, 5211-5219		6
323	Design space visualization for guiding investments in biodegradable and sustainably sourced materials. 2020 , 10, 18-24		1
322	Electron microscopy characterization of fast reactor MOX Joint Oxide-Gaine (JOG). <i>Journal of Nuclear Materials</i> , 2020 , 531, 151964	3.3	9
321	Synthesis and structural characterization of iron-cementite nanoparticles encapsulated in carbon matrix. 2020 , 22, 1		8
320	Bioimmobilization of toxic metals by precipitation of carbonates using <i>Sporosarcina luteola</i> : An in vitro study and application to sulfide-bearing tailings. 2020 , 724, 138124		11
319	Mechanism of Saponite Crystallization from a Rapidly Formed Amorphous Intermediate. 2020 , 20, 3365-3373		7
318	The CSD and knowledge databases: from answers to questions. 2020 , 22, 7298-7307		10

317	Quantum ESPRESSO toward the exascale. 2020 , 152, 154105	227
316	High-throughput computational materials screening and discovery of optoelectronic semiconductors. 2021 , 11,	19
315	Partial substitution of cement by the association of Ferronickel slags and Crepidula fornicata shells. 2021 , 33, 101587	12
314	Thermal behavior of Mg ₂ Ni-phyllsilicate nanoscrolls and performance of the resulting composites in hexene-1 and acetone hydrogenation. 2021 , 7, 257-269	1
313	Zinc oxide nanoparticle in lithium triborate microparticle system: Visibility for application in dosimetry. 2021 , 38, 879-886	2
312	Solid-State Thermal Control Devices. 2021 , 7, 2000625	11
311	Using molecular dynamics trajectories to predict nuclear spin relaxation behaviour in large spin systems. 2021 , 323, 106891	0
310	Early anthropogenic use of hematite on Aurignacian ivory personal ornaments from Hohle Fels and Vogelherd caves, Germany. 2021 , 150, 102900	3
309	BCL::Conf: Improved Open-Source Knowledge-Based Conformation Sampling Using the Crystallography Open Database. 2021 , 61, 189-201	3
308	Valence-to-core X-ray emission spectroscopy of titanium compounds using energy dispersive detectors. 2021 , 50, 9-20	8
307	Deep learning model for finding new superconductors. 2021 , 103,	11
306	Shifting computational boundaries for complex organic materials. 2021 , 17, 152-154	1
305	Influence of Plasma Nitriding with a Nitrogen Rich Gas Composition on the Reciprocating Sliding Wear of a DIN 18MnCrSiMo6-4 Steel. 2021 , 24,	2
304	Oxidation-assisted alkaline precipitation of nanoparticles using gas-diffusion electrodes. 2021 , 6, 1031-1041	
303	Peptide bond planarity constrains hydrogen bond geometry and influences secondary structure conformations. 2021 , 3, 1-8	2
302	Oriented Crystal Growth of La _{0.557} Li _{0.330} TiO ₃ in Bulk Ceramics Induced by LaAlO ₃ Single-Crystal Fibers. 2021 , 21, 2093-2100	
301	Validation of the Crystallography Open Database using the Crystallographic Information Framework. 2021 , 54, 661-672	36
300	Understanding Ring Puckering in Small Molecules and Cyclic Peptides. 2021 , 61, 743-755	9

299	Role of e-beam irradiation treatment on detemplation and structural hierarchy of ZSM-5 zeolite. 2021 , 315, 110928	3
298	How the Shape of Chemical Data Can Enable Data-Driven Materials Discovery. 2021 , 3, 111-119	3
297	: complexity and configurational entropy of crystal structures via information theory. 2021 , 54, 306-316	8
296	2D Materials Bridging Experiments and Computations for Electro/Photocatalysis. 2003841	35
295	Half-metallic ferromagnetism in layered CdOHCl induced by hole doping. 2021 , 8, 025027	3
294	Experimental and Simulation Analysis of Effects of Laser Bending on Microstructures Applied to Advanced Metallic Alloys. 2021 , 11, 362	
293	Development of spin-contrast-variation neutron powder diffractometry for extracting the structure factor of hydrogen atoms. 2021 , 54, 454-460	1
292	Deep learning in electron microscopy. 2021 , 2, 011004	14
291	Ultra-incompressible High-Entropy Diborides. 2021 , 12, 3106-3113	3
290	Understanding Conformational Entropy in Small Molecules. 2021 , 17, 2099-2106	6
289	Toward a High-Performance Aqueous Zinc Ion Battery: Potassium Vanadate Nanobelts and Carbon Enhanced Zinc Foil. 2021 , 21, 2738-2744	15
288	Geochemical signatures of lignite mining products in sediments downstream a fluvial-lacustrine system. 2021 , 760, 143942	4
287	Classification of beer by thermogravimetric and chemometric techniques. 1	
286	Morphological changes and kinetic assessment of Cu ₂ O powder reduction by non-thermal hydrogen plasma. 2021 , 11, 328-341	4
285	Growth Mechanisms of Nano-to Micro-Sized Lead Sulfate Particles. 2021 , 6, 10557-10567	1
284	Lab Case Study of Microbiologically Influenced Corrosion and Rietveld Quantitative Phase Analysis of X-ray Powder Diffraction Data of Deposits from a Refinery. 2021 , 6, 11822-11831	2
283	Enhancing deep-learning training for phase identification in powder X-ray diffractograms. 2021 , 8, 408-420	3
282	The stability analysis of the monolayer triangular borophene adsorbed on substrates: First-principles simulation. 2021 , 190, 110271	

281	Theoretical Prediction of Two-Dimensional Materials, Behavior, and Properties. 2021 , 15, 5959-5976		8
280	Synthesis and Crystal Structure of Some Ba-Apatites. 2021 , 66, 455-459		0
279	Atomic Properties of Monoclinic AgSe Thin Film Grown on SrTiO Substrate by Molecular Beam Epitaxy. 2021 , 12, 4140-4147		1
278	Silicon concentration and pH controls over competitive or simultaneous incorporation of iodate and chromate into calcium carbonate phases. 2021 , 128, 104941		0
277	One-pot synthesis of highly dispersed mesoporous Cu/ZrO ₂ catalysts for NH ₃ -SCR. 2021 ,		3
276	Interval support vector regression enables high-throughput machine learning predictions for dielectric constant of polymer dielectrics. 2021 , 118, 223901		2
275	synchrotron XRD measurements during solidification of a melt in the CaO-SiO ₂ system using an aerodynamic levitation system. 2021 , 33,		0
274	OCELOT: An infrastructure for data-driven research to discover and design crystalline organic semiconductors. 2021 , 154, 174705		5
273	The missing link: covalent linkages in structural models. 2021 , 77, 727-745		6
272	Geochemical investigations of noble metal-bearing ores: Synchrotron-based micro-analyses and microcosm bioleaching studies. 2021 , 270, 129388		1
271	Modal Analysis of Rock Forming Minerals: Contribution of XRD/Rietveld Analysis Compared to the Classic Point Counting Method. 2021 , 19, 395-413		2
270	Phase solubility diagrams and energy surface calculations support the solubility enhancement with low hygroscopicity of Bergenin: 4-Aminobenzamide (1: 1) cocrystal. 2021 , 601, 120537		5
269	Reactivity Effect of Calcium Carbonate on the Formation of Carboaluminate Phases in Ground Granulated Blast Furnace Slag Blended Cements. 2021 , 13, 6504		3
268	Tailoring growth modes by excess alkali addition in magnetron sputtered potassium sodium niobate thin films. 2021 , 27, 102221		2
267	Effect of the synthesis temperature on the phase composition of Al ₂ O ₃ . <i>Journal of Physics: Conference Series</i> , 2021 , 1942, 012052	0.3	1
266	Si ₃ N ₄ ceramics with sintering additive of MnO-TiO ₂ . <i>Journal of Physics: Conference Series</i> , 2021 , 1942, 012037	0.3	0
265	Dry sliding behaviour of composite friction materials with varying iron and copper content prepared using the spark plasma sintering technique. 1-13		2
264	Inorganic-based adsorbent materials for the removal of gaseous pollutants. 1		

263	Middle Stone Age mineral pigment procurement at Pinnacle Point 5â&#228 North, Western Cape province, South Africa.	0
262	Neutron Diffraction Study of a Sintered Iron Electrode In Operando. 2021 , 125, 16391-16402	0
261	Anisotropic thermal lattice expansion and crystallographic structure of strontium aluminide within Al-10Sr alloy as measured by in-situ neutron diffraction. 2021 , 869, 159232	0
260	Permeability and Mineralogy of the Jfalu Formation, Hungary, from Production Tests and Experimental Rock Characterization: Implications for Geothermal Heat Projects. 2021 , 14, 4332	2
259	Combinatorial growth of multinary nanostructured thin functional films. 2021 ,	3
258	Comparative Analysis of Recycled Plaster Composition Determined by X-ray Powder Diffraction and Thermogravimetric Analyses. 2021 , 1, 105-121	
257	Recent progress of the computational 2D materials database (C2DB). 2021 , 8, 044002	33
256	Interaction of silver nanoparticles with catechol methyltransferase: Spectroscopic and simulation analyses. 2021 , 26, 101013	1
255	Gallium Selenide Nanoribbons on Silicon Substrates for Photodetection. 2021 , 4, 7820-7831	2
254	Effects of polycarboxylate ether (PCE)-based superplasticizer on the dissolution and subsequent hydration of calcium oxide (CaO). 2021 , 146, 106467	1
253	Analysis of in vitro demineralised human enamel using multi-scale correlative optical and scanning electron microscopy, and high-resolution synchrotron wide-angle X-ray scattering. 2021 , 206, 109739	7
252	Adsorption of organic compounds from aqueous solution by pyridine-2-carboxaldehyde grafted MIL-101(Cr)-NH ₂ metal-organic frameworks. 2021 , 9, 105275	11
251	Ultra-low friction and edge-pinning effect in large-lattice-mismatch van der Waals heterostructures. 2021 ,	21
250	OPTIMADE, an API for exchanging materials data. <i>Scientific Data</i> , 2021 , 8, 217	8.2 8
249	Shear and Breathing Modes of Layered Materials. 2021 ,	4
248	Effect of MgO on the microstructure and properties of mullite membranes made by phase-inversion tape casting. 1-11	
247	Impact of Ca(II) on the aqueous speciation, redox behavior, and environmental mobility of Pu(IV) in the presence of EDTA. 2021 , 783, 146993	3
246	Crystal-Site-Based Artificial Neural Networks for Material Classification. 2021 , 11, 1039	0

245	Synthesis and Application of AgBiS and AgS Nanoinks for the Production of IR Photodetectors. 2021 , 6, 20710-20718		1
244	Complexity Parameters for Molecular Solids. 2021 , 13, 1399		5
243	Composite Pt/(SnO ₂ /C) and PtSnNi/C Catalysts for Oxygen Reduction and Alcohol Electrooxidation Reactions. 2021 , 57, 898-910		1
242	High temperature (up to 1200 °C) thermal-mechanical stability of Si and Ni doped CrN framework coatings. 2021 , 14, 2406-2419		1
241	Ferromagnetic L10-Structured CoPt Nanoparticles for Permanent Magnets and Low Pt-Based Catalysts. 2021 , 4, 9231-9240		0
240	The utility of composition-based machine learning models for band gap prediction. 2021 , 197, 110637		2
239	A preliminary investigation of a novel mortar based on alkali-activated seashell waste powder. 2021 , 389, 471-481		8
238	Structural dissection of sequence recognition and catalytic mechanism of human LINE-1 endonuclease. <i>Nucleic Acids Research</i> , 2021 , 49, 11350-11366	20.1	0
237	Applications of Machine Learning in Solid Oral Dosage Form Development. 2021 , 110, 3150-3165		5
236	Physicochemical characterization of monazite sand and its associated bacterial species from the beaches of southeastern Brazil. 2021 , 1		0
235	Factors Governing the Formation of Oxygen-Containing Copper Powders in a Plasma-Solution System. 1		0
234	Time dependent zero valent iron oxidation and the reductive removal of pertechnetate at variable pH. 2022 , 424, 127400		0
233	Synthesis and characterisation of alites from reduced basic oxygen furnace slags. 2021 , 147, 106518		1
232	Structural and magnetic properties of La-doped strontium-hexaferrites ceramics obtained by spark-plasma sintering. <i>Journal of Magnetism and Magnetic Materials</i> , 2021 , 533, 167966	2.8	2
231	An insight on the effect of sodium and silicon on microstructure and crystallography of high alumina cements. 2021 , 148, 106533		1
230	Elastic neutron scattering models for NCrystal. 2021 , 267, 108082		1
229	Adaptive global kernel interval SVR-based machine learning for accelerated dielectric constant prediction of polymer-based dielectric energy storage. 2021 , 176, 81-88		4
228	Effect of Biochar Filler on the Hydration Products and Microstructure in Portland Cement-stabilized Peat. 2021 , 33, 04021263		1

227	The crystal structure of Na ₂ CaAl ₄ O ₈ and its hydration behaviour. 2021 , 303, 122478	
226	Synthesis and properties of layered perovskite-like compounds PbBi ₂ Nb ₂ O ₉ and PbBi ₃ Ti ₂ NbO ₁₂ . 2021 , 121, 106730	1
225	Paramagnetic spin labeling of a bacterial DnaB helicase for solid-state NMR. 2021 , 332, 107075	1
224	Laterite and its potential as an alternative-bauxite. 2021 , 1, 100016	
223	Garnierite characterization for open mineral databases. 2021 , 231, 106874	1
222	Evaluation of thallium isotopic fractionation during the metallurgical processing of sulfides: An update. 2022 , 424, 127325	4
221	Is machine learning redefining the perovskite solar cells?. 2022 , 66, 74-90	5
220	Formation of highly dispersed tin nanoparticles in amorphous silicates for sodium ion battery anode. 2022 , 161, 110377	0
219	Accurate prediction of band gap of materials using stacking machine learning model. 2022 , 201, 110899	2
218	Thermal Analysis of Recycled Plastics. 2021 , 213-238	1
217	Assembling organic-inorganic building blocks for high-capacity electrode design. 2021 , 8, 1825-1834	1
216	Composites of Silicon@Li ₄ Ti ₅ O ₁₂ and Graphite for High-Capacity Lithium-Ion Battery Anode Materials. 2021 , 168, 010524	2
215	Measurements of Geologic Characteristics and Geophysical Properties of Sediments From the New England Mud Patch. 2021 , 1-28	6
214	Towards the object-oriented design of active hydrogen evolution catalysts on single-atom alloys. 2021 , 12, 10634-10642	4
213	Databases, Repositories, and Other Data Resources in Structural Biology. 2017 , 1607, 643-665	4
212	Machine Learning and Big-Data in Computational Chemistry. 2020 , 1939-1962	2
211	Oxidation states of iron as an indicator of the techniques used to burn clays and handcraft archaeological Tupiguarani ceramics by ancient human groups in Minas Gerais, Brazil. 2013 , 115-123	1
210	Acceleration of cement hydration from supplementary cementitious materials: Performance comparison between silica fume and hydrophobic silica. 2020 , 112, 103688	20

209	Combined powder metallurgy routes to improve thermal and mechanical response of Al ₃ Sn composite phase change materials. 2020 , 30, 3226-3239		4
208	Differentiating the Electrical and Optoelectrical Properties of Oxysulfides La ₂ Ta ₂ MS ₂ O ₈ (M = Zr, Ti) via Application of Pressure. 2020 , 124, 14477-14484		1
207	Synthesis and Characterization of Mixed-Valent Iron Layered Double Hydroxides (‘‘Green Rust’’). 2021 , 5, 40-54		4
206	Lanthanide Luminescence Enhancement of Core-Shell Magnetite-SiO ₂ Nanoparticles Covered with Chain-Structured Helical Eu/Tb Complexes. 2020 , 5, 32930-32938		5
205	Synthesis of oxygen-containing iron powders and water purification from iron ions by glow discharge of atmospheric pressure in contact with the solution. 2020 , 53, 445202		3
204	Importance of van der Waals interactions for ab initio studies of topological insulators. 2020 ,		3
203	Application of the Method of Statistical Comparison of XRD-and XRF-Data for Identification of the Most Representative Rock Samples: A Case Study of an Extensive Collection of Carbonatites and Aluminosilicate Rocks of the Kontozero Alkaline Complex (Kola Peninsula, NW Russia). 609, 012050		1
202	Warwick electron microscopy datasets. 2020 , 1, 045003		3
201	Age-related environmental gradients influence invertebrate distribution in the Prince Charles Mountains, East Antarctica. 2016 , 3, 160296		5
200	Towards novel organic high-T _c superconductors: Data mining using density of states similarity search. <i>Physical Review Materials</i> , 2018 , 2,	3.2	15
199	Machine learning in materials design and discovery: Examples from the present and suggestions for the future. <i>Physical Review Materials</i> , 2018 , 2,	3.2	57
198	Definition of a scoring parameter to identify low-dimensional materials components. <i>Physical Review Materials</i> , 2019 , 3,	3.2	12
197	Unsupervised landmark analysis for jump detection in molecular dynamics simulations. <i>Physical Review Materials</i> , 2019 , 3,	3.2	17
196	Minimum-strain symmetrization of Bravais lattices. 2020 , 2,		1
195	Accelerating k-nearest-neighbor searches. 2016 , 49, 1471-1477		2
194	Full-profile search-match by the Rietveld method. 2019 , 52, 587-598		21
193	Raman Open Database: first interconnected Raman-X-ray diffraction open-access resource for material identification. 2019 , 52, 618-625		18
192	Recent developments in the Inorganic Crystal Structure Database: theoretical crystal structure data and related features. 2019 , 52, 918-925		81

191	Validation and extraction of molecular-geometry information from small-molecule databases. 2017 , 73, 103-111	18
190	Nano and microcrystallites of KSbOSiO ₄ in glass matrix as a source of internal strain and fatal corrosion of historic turquoise glass. 2017 ,	3
189	Mineralogical and geochemical variation in stream sediments impacted by acid mine drainage is related to hydro-geomorphic setting. 2018 , 6,	4
188	The Effect of Firing Temperature on Structure and Electrical Properties in Low Temperature Co-fired Ceramics. 2016 , 2016, 000136-000141	3
187	<i></i></i></i></i></i></i> XAFS Characterization of PtPd Nanoparticles Synthesized by Galvanic Replacement. 2017 , 06, 75-91	3
186	Crystallography and Databases. 2017 , 16,	18
185	Terahertz study of L-asparagine and its monohydrate. 2014 , 63, 133203	3
184	Deep-Learning Estimation of Band Gap with the Reading-Periodic-Table Method and Periodic Convolution Layer. 2020 , 89, 124006	1
183	Cyanide Removal and Recovery by Electrochemical Crystallization Process. 2021 , 13, 2704	0
182	Salt-Water System under Diamond Confinement. 2021 , 125, 22283-22294	1
181	Crystal structure determination of a new LaPO ₄ phase in a multicomponent glass ceramic via 3D electron diffraction. 2021 , 48, 3790-3790	0
180	Formation of Pyrite Spherules From Mixtures of Biogenic FeS and Organic Compounds During Experimental Diagenesis. <i>Geochemistry, Geophysics, Geosystems</i> , 2021 , 22, e2021GC010056	3.6 0
179	A new magnetic composite with potential application in boron adsorption: Development, characterization, and removal tests. 2021 , 277, 125368	0
178	RCSB Protein Data Bank: Celebrating 50 years of the PDB with new tools for understanding and visualizing biological macromolecules in 3D. 2021 ,	11
177	Innovative Materials Science via Machine Learning. 2108044	9
176	Mud-Based Construction Material: Promising Properties of French Gravel Wash Mud Mixed with Byproducts, Seashells and Fly Ash as a Binder. 2021 , 14,	2
175	Applications of plasma synthesized ZnO, TiO ₂ , and Zn/TiO _x nanoparticles for making antimicrobial wound-healing viscose patches. e2100093	0
174	Molecular Dynamics Simulation of Sliding Friction Between Crystalline Cotton Fiber and Cr. 2021 , 69, 1	0

- 173 Diffusion in hypo-stoichiometric uranium mononitride. **2021**, 142, 103995
- 172 Parametric Rietveld Refinement Applied to In-Situ Monitoring of X-Ray Powder Diffraction Data of Plaster Hydration. **2019**, 22,
- 171 Encyclopedia of Big Data Technologies. **2019**, 358-365
- 170 Micro X-Ray Diffraction. **2019**, 427-439
- 169 Identification of the impurity phase in high-purity CeB by convergent-beam electron diffraction. **2019**, 75, 489-500 0
- 168 Iron rich self-assembly micelles on the Doce River continental shelf. **2021**, 151343
- 167 Thermodynamic properties of the Nd-Bi system via emf measurements, DFT calculations, machine learning, and CALPHAD modeling. **2021**, 223, 117448 3
- 166 Role of Mineralogy in Controlling Fracture Formation. 2
- 165 THERMOLUMINESCENCE AND KINETIC PARAMETERS OF MICRO-NANO MATRIX OF LITHIUM TRIBORATE AND ZINC OXIDE NANOPARTICLE. **2020**, 192, 430-443
- 164 Biogeochemical Controls on the Potential for Long-Term Contaminant Leaching from Soils Developing on Historic Coal Mine Spoil. **2021**, 5, 3 0
- 163 Geological Interpretation of the Results of Factor Analysis of XRF- and XRD-Data on Carbonatites and Aluminosilicate Rocks of the Kontozero Alkaline Complex (Kola Peninsula, NW Russia). 609, 012049
- 162 Crystallography Open Database (COD). **2020**, 1863-1881 2
- 161 Open-Science Platform for Computational Materials Science: AiiDA and the Materials Cloud. **2020**, 1813-1835 1
- 160 Microestrutura e Propriedades de Desgaste do Aço Bainítico de Resfriamento Contínuo DIN 18MnCrSiMo6-4 Nitretado a Plasma em Diferentes Temperaturas. **2020**, 25,
- 159 Casting synthesis of Bi₁₂SiO₂₀. **2021**, 31, 721-722 1
- 158 Iron in Hydroxyapatite: Interstitial or Substitution Sites?. **2021**, 11, 0
- 157 Predicting synthesizability of crystalline materials via deep learning. **2021**, 2, 3
- 156 The Impact of Redox, Hydrolysis and Dehydration Chemistry on the Structural and Magnetic Properties of Magnetoferritin Prepared in Variable Thermal Conditions. **2021**, 26,

155	Upcycling Waste Plastics into Multi-Walled Carbon Nanotube Composites via NiCo ₂ O ₄ Catalytic Pyrolysis. 2021 , 11, 1353		0
154	Mineralogy of Ga- and Ge-bearing metallurgical slags from Tsumeb (Namibia). 1-34		1
153	Plasma-solution synthesis of particles containing transition metals. <i>Journal of Physics: Conference Series</i> , 2021 , 2064, 012096	0.3	0
152	The proof-of-concept of a novel feces destroyer latrine. 2021 , 10, 106827		3
151	Morphology, mineralogy and rietveld texture analysis of ash deposits from a moving grate boiler. 2021 , 314, 122737		0
150	Nanocomposite of graphene and WO ₃ nanowires for carbon monoxide sensors. 2021 , 7, 225-236		0
149	Hydrostatic compression and pressure phase transition of major Portland cement constituents – Insights via molecular dynamics modeling. 2022 , 7, 100017		
148	Characterisation and leaching behavior of CaO-modified iron-silicate slag produced in laboratory and industrial scales. 2021 , 60, 294-305		0
147	Nanocrystalline rhenium-doped TiO ₂ : an efficient catalyst in the one-pot conversion of carbohydrates into levulinic acid. The synergistic effect between Brønsted and Lewis acid sites. 2022 , 12, 167-180		0
146	Structural Properties and Magnetic Ground States of 100 Binary -Metal Oxides Studied by Hybrid Density Functional Methods.. 2022 , 27,		1
145	Microstructure and Wear Properties of a Low Carbon Bainitic Steel on Plasma Nitriding at Different N ₂ -H ₂ Gas Mixtures. 25,		1
144	The mineralogical composition of coarse and fine particulate material, their fate, and sources in an industrialized region of southeastern Brazil.. 2022 , 194, 88		1
143	Evaluation of Stereolithography-Based Additive Manufacturing Technology for BaTiO ₃ Ceramics at 465 nm. 2022 , 12, 412		1
142	Mechanistic Understanding of DNA Denaturation in Nanoscale Thermal Gradients Created by Femtosecond Excitation of Gold Nanoparticles.. <i>ACS Applied Materials & Interfaces</i> , 2022 ,	9.5	0
141	High-Latitude Paleointensities During the Cretaceous Normal Superchron From the Okhotsk-Chukotka Volcanic Belt. 2022 , 127,		0
140	Enhancement of thermal and mechanical stabilities of silicon doped titanium nitride coating by manipulation of sputtering conditions. 2022 , 17, 1122-1131		2
139	Formation of Silicon Nanoclusters in Disproportionation of Silicon Monoxide. 2021 , 55, 423		1
138	Smart Materials Prediction: Applying Machine Learning to Lithium Solid-State Electrolyte.. 2022 , 15,		1

137	Chemical composition data-driven machine-learning prediction for phase stability and materials properties of inorganic crystalline solids.	
136	Observation of gunpowder-like thermochemical responses of a thermal energy storage system based on KNO ₃ /NaNO ₃ /Graphite exposed to a heat transfer fluid. 2022 , 207, 118215	0
135	A strategic review of MXenes as emergent building blocks for future two-dimensional materials: recent progress and perspectives. 2022 , 10, 4096-4123	2
134	Teaching basic crystallography and diffraction using open access structure visualization software. 1	0
133	A review of the recent progress in battery informatics. 2022 , 8,	4
132	Investigation of the effect of sintering temperature on structural, magnetic and magnetocaloric properties in PrCaMn ₂ O ₆ double perovskite manganite system. 2022 , 33, 7357-7370	0
131	Black Fungi and Stone Heritage Conservation: Ecological and Metabolic Assays for Evaluating Colonization Potential and Responses to Traditional Biocides. 2022 , 12, 2038	4
130	Updated restraint dictionaries for carbohydrates in the pyranose form.. 2022 , 78, 455-465	0
129	Graph-based machine learning beyond stable materials and relaxed crystal structures. <i>Physical Review Materials</i> , 2022 , 6,	3.2
128	Advanced perspectives in the EXPO software for solving crystal structures from powder diffraction data. 2022 , 55, 411-419	0
127	Manufacturing of Textured Bulk Fe-SmCo Magnets by Severe Plastic Deformation.. 2022 , 12,	
126	A Workflow Demonstrator for Processing Catalysis Research Data. 1-16	1
125	Realization of a cost-effective thermochromic solar absorber with a high emittance change based on VO ₂ and an infrared transparent intermediate layer. 2022 , 12, 035118	
124	Robust Design of High-Performance Optoelectronic Chalcogenide Crystals from High-Throughput Computation.. 2022 ,	4
123	Improvement of cob thermal inertia by latent heat storage and its implication on energy consumption. 2022 , 329, 127163	2
122	Making the collective knowledge of chemistry open and machine actionable.. 2022 , 14, 365-376	2
121	Cobalt-bearing copper slags from Luanshya (Zambian Copperbelt): Mineralogy, geochemistry, and potential recovery of critical metals. 2022 , 237, 106987	2
120	Synthesis and characterization of Fe ₂ O ₃ -TiO ₂ magnetic materials: Effect of heat-treatment on catalytic activity of naphthalene hydrogenation. 2022 , 392-393, 167-179	0

119	Effect of peat organic matter on sulfide weathering and thallium reactivity: Implications for organic environments.. 2022 , 299, 134380	0
118	Gram-Scale Synthesis of CoO/C as Base for PtCo/C High-Performance Catalysts for the Oxygen Reduction Reaction. 2021 , 11, 1539	1
117	Elasticity-based-exfoliability measure for high-throughput computational exfoliation of two-dimensional materials. 2021 , 7,	2
116	Characterisation and leaching behaviour of granulated iron silicate slag constituents. 2022 , 61, 14-23	0
115	COPEX: co-evolutionary crystal structure prediction algorithm for complex systems. 2021 , 7,	3
114	Forming mechanism of equilibrium and non-equilibrium metallurgical phases in dissimilar aluminum/steel (Al-Fe) joints.. 2021 , 11, 24251	1
113	Preparation of Cu/ZrW ₂ O ₈ structures by chemical deposition from formaldehyde-free solution. 2022 , 100, 18-24	1
112	Instability of Ga-substituted Li ₇ La ₃ Zr ₂ O ₁₂ toward Metallic Li.	4
111	Self-flux-grown Ba ₄ Fe ₄ ClO _{9.5} crystals exhibiting structures with tunable modulation.	
110	Intermediate polaronic charge transport in organic crystals from a many-body first-principles approach. 2022 , 8,	2
109	From the Periodic Properties of Metals to the Rietveld Refinement of the Pharmaceutical Molecule Naproxen: Three Remote Experiments about X-ray Diffraction.	1
108	Variations in the mineral structures dominating solute mobilization during clay compaction. 2022 , 127843	0
107	Facile Production of CsPbBr ₃ Perovskite Single-Crystals in a Hydrobromic Solution.	
106	Structure, Properties, and Phase Transformations of Water Nanoconfined between Brucite-like Layers: The Role of Wall Surface Polarity.. 2022 , 15,	
105	Improvement on pitting wear resistance of gears by controlled forging and plasma nitriding. 2022 , 18, 4698-4713	0
104	High-Throughput Discovery and Investigation of Auxetic Two-Dimensional Crystals.	0
103	Micro-Raman Spectroscopy and X-ray Diffraction Analyses of the Core and Shell Compartments of an Iron-Rich Fulgurite. 2022 , 27, 3053	
102	Soils of the coastal and lower belt of Galápagos Islands –The case of Isla Santa F and Isla Santa Cruz. 2022 , 29, e00520	

101	Direct space approach in action: Challenging structure solution of microcrystalline materials using the EXPO software. 2022 , 210, 111465		
100	Energy storage performance of polycrystalline Bi _{0.85} Ho _{0.05} Sm _{0.1} FeO ₃ ceramics. 2022 , 589, 55-63	1	
99	Challenges in Information-Mining the Materials Literature: A Case Study and Perspective.	0	
98	Iron-cementite nanoparticles in carbon matrix: Synthesis, structure and magnetic properties. <i>Journal of Magnetism and Magnetic Materials</i> , 2022 , 169503	2.8	
97	Magnetoactive elastomers based on ferromagnetic and ferroelectric particles: A FORC approach. <i>Journal of Magnetism and Magnetic Materials</i> , 2022 , 558, 169506	2.8	1
96	Assessment of software for the analysis of electron diffraction patterns obtained by transmission electron microscopy and modelling. 2022 ,		
95	Development of RuS ₂ for near-infrared photodetector by atomic layer deposition and post-sulfurization.		
94	The Effect of Zn Content and Granulation Temperature on Zn Leaching in an Fe-Saturated (FeXZn(1- λ)) ₂ SiO ₄ System. <i>Minerals (Basel, Switzerland)</i> , 2022 , 12, 767	2.4	
93	Effect of bond valence sum on the structural modeling of lead borate glass. <i>Journal of Non-Crystalline Solids</i> , 2022 , 121751	3.9	0
92	Novel inorganic crystal structures predicted using autonomous simulation agents. <i>Scientific Data</i> , 2022 , 9,	8.2	0
91	Inorganic Crystal Structure Prototype Database Based on Unsupervised Learning of Local Atomic Environments. <i>Journal of Physical Chemistry A</i> ,	2.8	1
90	The crystal structure and transformations of the omicron phase ϵ in the Ti-Al-Nb system and on the ambiguity of its subvariants ϵ_1 and ϵ_2 . <i>Scripta Materialia</i> , 2022 , 219, 114841	5.6	0
89	Microscopic Molecular Insights into Methane Hydrate Growth on the Surfaces of Clay Minerals: Experiments and Molecular Dynamics Simulations. <i>SSRN Electronic Journal</i> ,	1	
88	New challenges in oxygen reduction catalysis: a consortium retrospective to inform future research. <i>Energy and Environmental Science</i> ,	35.4	1
87	Computational exfoliation of atomically thin one-dimensional materials with application to Majorana bound states. <i>Physical Review Materials</i> , 2022 , 6,	3.2	0
86	Crystal Growth of Urea and Its Modulation by Additives as Analyzed by All-Atom MD Simulation and Solution Theory. <i>Journal of Physical Chemistry B</i> ,	3.4	
85	Effect of microbial-induced calcite precipitation towards strength and permeability of peat. <i>Bulletin of Engineering Geology and the Environment</i> , 2022 , 81,	4	
84	The effect of high-temperature nanoparticle-based modification on the structure of zinc oxide powders. <i>Journal of Physics: Conference Series</i> , 2022 , 2291, 012019	0.3	

83	Toward Automated Computational Discovery of Battery Materials. <i>Advanced Materials Technologies</i> , 2200616	6.8	2
82	Data format standards in analytical chemistry. <i>Pure and Applied Chemistry</i> , 2022 ,	2.1	0
81	Leveraging computational thermodynamics to guide SiC-ZrC chemical vapor deposition process development. <i>Surface and Coatings Technology</i> , 2022 , 444, 128672	4.4	1
80	Thermodynamic investigations of the LiF-CsF and NaF-CsF pseudo-binary systems. <i>Journal of Nuclear Materials</i> , 2022 , 568, 153901	3.3	
79	Effects of flow on uranium speciation in soils impacted by acidic waste fluids. <i>Journal of Environmental Radioactivity</i> , 2022 , 251-252, 106955	2.4	
78	Black TiO ₂ Photoanodes for Direct Methanol Photo Fuel Cells. <i>ACS Applied Materials & Interfaces</i> ,	9.5	0
77	Application of Molecular-Modeling, Scaffold-Hopping, and Bioisosteric Approaches to the Discovery of New Heterocyclic Picolinamides. <i>Journal of Agricultural and Food Chemistry</i> ,	5.7	0
76	Greigite (Fe ₃ S ₄) formation in artificial sediments via solid-state transformation of lepidocrocite. <i>Geochemistry, Geophysics, Geosystems</i> ,	3.6	0
75	Insight into ground-state spin arrangement and bipartite entanglement of the polymeric coordination compound [Dy ₂ Cu ₂]. <i>Journal of Magnetism and Magnetic Materials</i> , 2022 , 561, 169721	2.8	0
74	Hydrothermal Synthesis of Hydrosilicate Nanoscrolls (Mg _{1-x} Cox) ₃ Si ₂ O ₅ (OH) ₄ in a Na ₂ SO ₃ Solution. 2022 , 67, 839-849		
73	Machine learning aided synthesis and screening of HER catalyst: Present developments and prospects. 1-31		0
72	Investigation of the Implementation of Laser Surface Alloying of Cu with CrWC. 2022 , 15, 5396		
71	Physico-chemical properties of waste derived biochar from community scale faecal sludge treatment plants. 6, 96		1
70	Investigation of Mechanical and Thermal Performance of Concrete with Scallop Shells as Partial Cement Replacement: Alternative Binder and Life Cycle Assessment. 2022 , 3, 760-778		0
69	Machine Learning: A New Paradigm in Computational Electrocatalysis. 7920-7930		5
68	Improving Material Property Prediction by Leveraging the Large-Scale Computational Database and Deep Learning.		
67	Microscopic molecular insights into methane hydrate growth on the surfaces of clay minerals: Experiments and molecular dynamics simulations. 2022 , 138757		0
66	Prediction of Solubility and Miscibility Parameters of Bismuth-Arsenic Complex and Amorphous Mineral Compounds Using Molecular Dynamics Simulation.		

65	Investigation of structural, optical and magnetic properties of $Y_{3-x}Ce_xFe_5-yEr_yO_{12}$ compound. 2022 , 644, 414231	0
64	Toxicity and decontamination strategies of Congo red dye. 2022 , 19, 100844	1
63	On the value of popular crystallographic databases for machine learning prediction of space groups. 2022 , 240, 118353	0
62	Spark plasma sintered, MoNbTi-based multi-principal element alloys with Cr, V, and Zr. 2022 , 927, 167083	0
61	Visualising coke-induced degradation of catalysts used for CO ₂ -reforming of methane with X-ray nano-computed tomography. 2022 , 5, 100068	0
60	Ambient-pressure ozone treatment enables tuning of oxygen vacancy concentration in the $La_{1-x}Sr_xFeO_{3-\delta}$ perovskite oxides.	0
59	Marine Biofilm effect on mortar surface layer.. 2022 , 1245, 012014	0
58	STRUCTURAL COMPLEXITY OF POLYMORPHS OF CALCIUM CARBONATE AND ITS CRYSTALLINE HYDRATES. 2022 , 63, 1291-1303	0
57	Energetic Stability and Interfacial Complexity of Ti ₃ C ₂ T _x MXenes Synthesized with HF/HCl and CoF ₂ /HCl as Etching Agents. 2022 , 14, 41542-41554	0
56	Electronic Configurations of 3d Transition-Metal Compounds Using Local Structure and Neural Networks.	1
55	Bond-length distributions in ionically bonded materials with decomposition by coordination environment. 2022 , 55, 1359-1367	0
54	Machine learning in electron microscopy for advanced nanocharacterization: current developments, available tools and future outlook.	1
53	Rapid and efficient room-temperature serial synchrotron crystallography using the CFEL TapeDrive. 2022 , 9, 778-791	0
52	Machine-learning accelerated identification of exfoliable two-dimensional materials.	0
51	Role of the Potential Range during Stress Testing of Platinum-Containing Electrocatalysts at Elevated Temperature. 2022 , 12, 1179	1
50	Analytical approaches in the development of industry standard specimens of aluminum production electrolyte. 2022 , 88, 20-29	0
49	Contaminant binding and bioaccessibility in the dust from the Ni-Cu mining/smeltering district of Selebi-Phikwe (Botswana).	0
48	Abundance of Second Order Topology in C ₃ Symmetric Two-dimensional Insulators.	0

- 47 Synthesis, characterization and energy gap of silica quantum dots from rice husk. **2022**, 20, 101263 ○
- 46 Gallium and germanium extraction and potential recovery from metallurgical slags. **2022**, 379, 134677 1
- 45 FAIR Big Data in the Materials Design Domain. **2022**, 1-8 ○
- 44 Superconductivity information extraction from the literature: A new corpus and its evaluations. **2022**, 54, 101768 ○
- 43 Integrating in-bed gas looping and CO₂ capture in the FeD-Latrline. **2022**, 160133 ○
- 42 Long-Term Leaching Effects on CaO-Modified Iron Silicate Slag. **2022**, 12, 1442 ○
- 41 Machine learning-driven design of promising perovskites for photovoltaic applications: A review. **2022**, 35, 102470 ○
- 40 Effects of pH on Ice Nucleation by the α -Alumina (0001) Surface. ○
- 39 First-principles Phonon Calculations with Phonopy and Phono3py. **2023**, 92, ○
- 38 Pore formation mechanism and intermetallic phase transformation in Ti- α Al alloy during reactive sintering. **2023**, 22, 1878-1887 ○
- 37 Engineering crystal water in potassium ammonium vanadate for fast Zn-ion storage. ○
- 36 Reductive removal of pertechnetate and chromate by zero valent iron under variable ionic strength conditions. **2023**, 445, 130546 ○
- 35 Influence of pH on Ice Nucleation by Kaolinite: Experiments and Molecular Simulations. **2022**, 126, 9227-9243 ○
- 34 Band-gap assessment from X-ray powder diffraction using artificial intelligence. **2022**, 55, 1538-1548 ○
- 33 Influence of caprolactam on the tin electrodeposition on a dispersed carbon support and preparation of Pt/(SnO₂/C) catalysts. **2022**, 2, ○
- 32 Physico-chemical properties of waste derived biochar from community scale faecal sludge treatment plants. 6, 96 ○
- 31 Effective Method for the Determination of the Unit Cell Parameters of New MXenes. **2022**, 15, 8798 ○
- 30 Printable high-efficiency organic ionic photovoltaic materials discovered by high-throughput first-principle calculations. **2022**, 25, 105639 ○

- 29 Phase analysis of simulated nuclear fuel debris synthesized using UO₂, Zr, and stainless steel and leaching behavior of the fission products and matrix elements. **2022**, ○
- 28 Graph-Convolutional Neural Net Model of the Statistical Torsion Profiles for Small Organic Molecules. **2022**, 62, 5896-5906 ○
- 27 Characterization of Mortar from Casa Barbot (Portugal), a Case Study from the Beginning of the 20th Century. **2023**, 13, 232 1
- 26 Investigation of the mechanical and hygrothermal behavior of coffee ground wastes valorized as a building material: analysis of mix designs performance and sorption curve linearization effect. **2023**, 23, 1 ○
- 25 Investigation of the metastable spinodally decomposed magnetic CrFe-rich phase in Al doped CrFeCoNi alloy. **2023**, 939, 168794 ○
- 24 Enhanced photocatalytic detoxication properties of OV-rich Pd/NiTiO₂ heterojunctions: excellent charge separation and mechanism insight. **2023**, 28, 101358 ○
- 23 A secured big-data sharing platform for materials genome engineering: State-of-the-art, challenges and architecture. **2023**, 142, 59-74 ○
- 22 Use of Biomass Ash in Reinforced Clayey Soil: A Multiscale Analysis of Solid-State Reactions. **2023**, 8, 5 ○
- 21 Association of Keplerate-Type Polyoxometalate {Mo₇₂Fe₃₀} with Tetracycline: Nature of Binding Sites and Antimicrobial Action. **2023**, 11, 9 ○
- 20 Introduction to perovskites. **2023**, 3-29 ○
- 19 Mixed Valence of Bismuth in Hexagonal Chalcogenide Nanocrystals. ○
- 18 Hundreds of new, stable, one-dimensional materials from a generative machine learning model. **2023**, 7, ○
- 17 Inter-quintuple layer coupling and topological phase transitions in the chalcogenide topological insulators. **2023**, 5, 015001 ○
- 16 Role of phosphorous in transition metal phosphides for selective hydrogenolysis of hindered C=O bonds. **2023**, 421, 403-418 ○
- 15 Characterisation of residual stresses and oxides in titanium, nickel, and aluminium alloy additive manufacturing powders via synchrotron X-ray diffraction. **2023**, 35, 105900 ○
- 14 Coexistence of Sn and FeSn₂ nanoparticles dispersed in glass-ceramics and their electrochemical performance as sodium-ion battery anode. **2023**, 947, 169576 ○
- 13 In situ ligand restraints from quantum-mechanical methods. **2023**, 79, 100-110 ○
- 12 Investigation of the hydration process and biological activity of a novel nanosilver incorporated dicalcium silicate based retrograde filling material. 11, e14632 ○

- 11 On the Subset of Intermolecular Contacts Generating a Molecular Crystal: Topological Features of Organic Minerals. **2022**, 67, 1133-1145 ○
- 10 Graph isomorphism-based algorithm for cross-checking chemical and crystallographic descriptions. **2023**, 15, 1
- 9 CrystalMELA: a new crystallographic machine learning platform for crystal system determination. **2023**, 56, 409-419 ○
- 8 Synthesis and characterization of bismuth ferrite particles using a nano-agitator bead mill. **2023**, 13, 035004 ○
- 7 Nanowires exfoliated from one-dimensional van der Waals transition metal trihalides and quadrihalides. **2023**, 5, 2096-2101 ○
- 6 Optical, electrical, structural, and morphological properties of $KAl_4Si_2O_{12}/Mg_3Si_2O_9/Fe_2O_3$ clay mineral from Machado mountain region, Tarairí Colombia. **2022**, 13, 43-55 ○
- 5 Catalogue of phonon modes in several cuprate high-temperature superconductors from density functional theory. **2023**, 6, ○
- 4 Exploitation of the Concept of Vicariance to Predict the Space Group of Lithiated Manganese or Cobalt Oxides. **2023**, 13, 602 ○
- 3 Characterisation of Secondary Copper Smelting Slag With Transmission Electron Microscopy. ○
- 2 Beyond Lattice Matching: The Role of Hydrogen Bonding in Epitaxial Nucleation of Poly(hydroxyalkanoates) by Methylxanthines. ○
- 1 Exploring the Possibility of Machine Learning for Predicting Ionic Conductivity of Solid-State Electrolytes. **2023**, 8, 16419-16427 ○