Janine George

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1872092/publications.pdf

Version: 2024-02-01

		394286	345118
40	1,321	19	36
papers	citations	h-index	g-index

59	59	59	1361
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	<scp>LOBSTER</scp>: Local orbital projections, atomic charges, and chemicalâ€bonding analysis from <scp>projectorâ€augmentedâ€waveâ€based</scp> densityâ€functional theory. Journal of Computational Chemistry, 2020, 41, 1931-1940.	1.5	523
2	Cooperativity of Halogen, Chalcogen, and Pnictogen Bonds in Infinite Molecular Chains by Electronic Structure Theory. Journal of Physical Chemistry A, 2014, 118, 3193-3200.	1.1	90
3	The Limited Predictive Power of the Pauling Rules. Angewandte Chemie - International Edition, 2020, 59, 7569-7575.	7.2	49
4	Plane-Wave Density Functional Theory Meets Molecular Crystals: Thermal Ellipsoids and Intermolecular Interactions. Accounts of Chemical Research, 2017, 50, 1231-1239.	7.6	47
5	Uncovering design principles for amorphous-like heat conduction using two-channel lattice dynamics. Materials Today Physics, 2021, 18, 100344.	2.9	42
6	Chemist versus Machine: Traditional Knowledge versus Machine Learning Techniques. Trends in Chemistry, 2021, 3, 86-95.	4.4	36
7	Î²â€CuN₃: The Overlooked Groundâ€State Polymorph of Copper Azide with Heterographeneâ€Like Layers. Angewandte Chemie - International Edition, 2015, 54, 1954-1959.	7.2	30
8	The Limited Predictive Power of the Pauling Rules. Angewandte Chemie, 2020, 132, 7639-7645.	1.6	30
9	Combining phonon accuracy with high transferability in Gaussian approximation potential models. Journal of Chemical Physics, 2020, 153, 044104.	1.2	29
10	High-throughput computational discovery of In2Mn2O7 as a high Curie temperature ferromagnetic semiconductor for spintronics. Npj Computational Materials, 2019, 5, .	3.5	28
11	Exploring the Origins of Improved Photocurrent by Acidic Treatment for Quaternary Tantalum-Based Oxynitride Photoanodes on the Example of CaTaO₂N. Journal of Physical Chemistry C, 2020, 124, 152-160.	1.5	28
12	Oxygen-Storage Materials BaYMn2O5+Î´ from the Quantum-Chemical Point of View. Chemistry of Materials, 2012, 24, 1910-1916.	3.2	27
13	Anisotropic displacement parameters from dispersion-corrected DFT methods and their experimental validation by temperature-dependent X-ray diffraction. CrystEngComm, 2015, 17, 7414-7422.	1.3	27
14	Considering the Role of Ion Transport in Diffusonâ€Dominated Thermal Conductivity. Advanced Energy Materials, 2022, 12, .	10.2	27
15	High-throughput computational search for high carrier lifetime, defect-tolerant solar absorbers. Energy and Environmental Science, 2021, 14, 5057-5073.	15.6	23
16	Significant Lanthanoid Substitution Effect on the Redox Reactivity of the Oxygen-Storage Material BaYMn₂O_{5+Î´}. Chemistry of Materials, 2016, 28, 4409-4414.	3.2	21
17	ChemEnv: a fast and robust coordination environment identification tool. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 683-695.	0.5	21
18	On the DFT Ground State of Crystalline Bromine and Iodine. ChemPhysChem, 2015, 16, 728-732.	1.0	20

#	Article	IF	Citations
19	Lattice thermal expansion and anisotropic displacements in ?-sulfur from diffraction experiments and first-principles theory. Journal of Chemical Physics, 2016, 145, 234512.	1.2	19
20	Dimensionality of Intermolecular Interactions in Layered Crystals by Electronic-Structure Theory and Geometric Analysis. Inorganic Chemistry, 2015, 54, 956-962.	1.9	18
21	Intermolecular contacts in bromomalonic aldehydeâ€"intuition, experiment, and theory. CrystEngComm, 2014, 16, 135-138.	1.3	17
22	Ammonothermal Synthesis, Crystal Structure, and Properties of the Ytterbium(II) and Ytterbium(III) Amides and the First Two Rare-Earth-Metal Guanidinates, YbC(NH)₃ and Yb(CN₃H₄)₃. Inorganic Chemistry, 2016, 55, 6161-6168.	1.9	17
23	Synthesis, Crystal Structure, Polymorphism, and Magnetism of Eu(CN3H4)2 and First Evidence of EuC(NH)3. Inorganics, 2017, 5, 10.	1.2	17
24	Lattice thermal expansion and anisotropic displacements in urea, bromomalonic aldehyde, pentachloropyridine, and naphthalene. Journal of Chemical Physics, 2017, 147, 074112.	1.2	16
25	Anisotropic thermal motion in transition-metal carbonyls from experiments and ab initio theory. Dalton Transactions, 2016, 45, 13680-13685.	1.6	15
26	Tetrel Bonds in Infinite Molecular Chains by Electronic Structure Theory and Their Role for Crystal Stabilization. Journal of Physical Chemistry A, 2017, 121, 1381-1387.	1.1	15
27	Automated Bonding Analysis with Crystal Orbital Hamilton Populations. ChemPlusChem, 2022, 87, .	1.3	15
28	The many flavours of halogen bonds â€“ message from experimental electron density and Raman spectroscopy. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 1190-1201.	0.2	14
29	Synthesis, Structure, and Properties of SrC(NH)₃, a Nitrogenâ€Based Carbonate Analogue with the Trinacria Motif. Angewandte Chemie - International Edition, 2015, 54, 12171-12175.	7.2	12
30	Ferroelectricity and multiferroicity in antiâ€“Ruddlesdenâ€“Popper structures. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	9
31	Synthesis, Structure Determination and Electronic Structure of Magnesium Nitride Chloride, Mg₂NCl. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2015, 641, 266-269.	0.6	7
32	Automation in DFT-based computational materials science. Trends in Chemistry, 2021, 3, 697-699.	4.4	6
33	A new tool for validating theoretically derived anisotropic displacement parameters with experiment: directionality of prolate displacement ellipsoids. CrystEngComm, 2019, 21, 6396-6404.	1.3	4
34	First Full Structural Characterization of Chloro Formamidinium Salts. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2018, 644, 1485-1491.	0.6	1
35	Das Rezept fÃ¼r schmalbandige Leuchtstoffe. Nachrichten Aus Der Chemie, 2020, 68, 54-58.	0.0	1
36	Die Materialsynthesemaschine. Nachrichten Aus Der Chemie, 2020, 68, 66-69.	0.0	1

#	Article	IF	Citations
37	UngewÃ¶hnliche Oxidationsstufen, (un)gewÃ¶hnliche MaÃŸnahmen. Nachrichten Aus Der Chemie, 2021, 69, 73-78.	0.0	0
38	Neue Materialien vorhersagen: Maschinelles Lernen als Werkzeug. Nachrichten Aus Der Chemie, 2020, 68, 49-52.	0.0	0
39	Vorhersagen aus Hochdurchsatzstudien. Nachrichten Aus Der Chemie, 2020, 68, 80-83.	0.0	0
40	Temperatur mit Licht messen. Nachrichten Aus Der Chemie, 2020, 68, 68-73.	0.0	0