

Josef W Zwanziger

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/2394250/publications.pdf>

Version: 2024-02-01

115
papers

7,773
citations

117625

34
h-index

49909

87
g-index

118
all docs

118
docs citations

118
times ranked

8134
citing authors

#	ARTICLE	IF	CITATIONS
1	ABINIT: First-principles approach to material and nanosystem properties. <i>Computer Physics Communications</i> , 2009, 180, 2582-2615.	7.5	2,297
2	Recent developments in the ABINIT software package. <i>Computer Physics Communications</i> , 2016, 205, 106-131.	7.5	662
3	Crystal and Electronic Structures of Complex Bismuth Iodides $\text{A}_3\text{Bi}_2\text{I}_9$ ($\text{A} = \text{K}, \text{Rb}, \text{Cs}$) Related to Perovskite: Aiding the Rational Design of Photovoltaics. <i>Chemistry of Materials</i> , 2015, 27, 7137-7148.	6.7	413
4	The Abinitproject: Impact, environment and recent developments. <i>Computer Physics Communications</i> , 2020, 248, 107042.	7.5	369
5	Fractional Quantization of Molecular Pseudorotation in Na_3 . <i>Physical Review Letters</i> , 1986, 56, 2598-2601.	7.8	293
6	Oxygen-17 NMR in solids by dynamic-angle spinning and double rotation. <i>Nature</i> , 1989, 339, 42-43.	27.8	244
7	ABINIT: Overview and focus on selected capabilities. <i>Journal of Chemical Physics</i> , 2020, 152, 124102.	3.0	179
8	Structure, Mobility, and Interface Characterization of Self-Organized Organic-Inorganic Hybrid Materials by Solid-State NMR. <i>Journal of the American Chemical Society</i> , 1999, 121, 5727-5736.	13.7	156
9	Short-and Intermediate-Range Structural Ordering in Glassy Boron Oxide. <i>Science</i> , 1995, 269, 1416-1420.	12.6	132
10	Topological phase in molecular bound states: Application to the $\text{Ea}^{\text{S}}-\text{e}$ system. <i>Journal of Chemical Physics</i> , 1987, 87, 2954-2964.	3.0	125
11	Multiple boron sites in borate glass detected with dynamic angle spinning nuclear magnetic resonance. <i>Journal of Non-Crystalline Solids</i> , 1994, 168, 293-297.	3.1	125
12	Platinum-Containing Hyper-Cross-Linked Polystyrene as a Modifier-Free Selective Catalyst for l-Sorbose Oxidation. <i>Journal of the American Chemical Society</i> , 2001, 123, 10502-10510.	13.7	116
13	A silica sol-gel design strategy for nanostructured metallic materials. <i>Nature Materials</i> , 2012, 11, 460-467.	27.5	112
14	Structural investigation of bismuth borate glasses and crystalline phases. <i>Journal of Non-Crystalline Solids</i> , 2009, 355, 45-53.	3.1	102
15	Network Modification in Potassium Borate Glasses: Structural Studies with NMR and Raman Spectroscopies. <i>The Journal of Physical Chemistry</i> , 1996, 100, 16720-16728.	2.9	99
16	The Structure of Alkali Tellurite Glasses. <i>Journal of Physical Chemistry B</i> , 2001, 105, 67-75.	2.6	99
17	Theoretical aspects of higher-order truncations in solid-state nuclear magnetic resonance. <i>Journal of Chemical Physics</i> , 1992, 97, 8947-8960.	3.0	98
18	Zero Thermal Expansion in $\text{ZrMgMo}_3\text{O}_{12}$: NMR Crystallography Reveals Origins of Thermoelastic Properties. <i>Chemistry of Materials</i> , 2015, 27, 2633-2646.	6.7	90

#	ARTICLE	IF	CITATIONS
19	Nanostructured Inorganic-Organic Composites as a Basis for Solid Polymer Electrolytes with Enhanced Properties. Chemistry of Materials, 2001, 13, 3678-3684.	6.7	84
20	Temperature dependent lattice misfit and coherency of Al ₃ X (X = Sc, Zr, Ti and Nb) particles in an Al matrix. Acta Materialia, 2015, 89, 109-115.	7.9	80
21	The structure of tellurite glass: a combined NMR, neutron diffraction, and X-ray diffraction study. Journal of Non-Crystalline Solids, 2000, 274, 1-8.	3.1	79
22	Zero-Stress Optic Glass without Lead. Chemistry of Materials, 2007, 19, 286-290.	6.7	67
23	Phonon dispersion and Grüneisen parameters of zinc dicyanide and cadmium dicyanide from first principles: Origin of negative thermal expansion. Physical Review B, 2007, 76, .	3.2	62
24	Measuring the geometric component of the transition probability in a two-level system. Physical Review A, 1991, 43, 3232-3240.	2.5	60
25	Design of organic-inorganic solid polymer electrolytes: synthesis, structure, and properties. Journal of Materials Chemistry, 2004, 14, 1812-1820.	6.7	51
26	The ring structure of boron trioxide glass. Journal of Non-Crystalline Solids, 2000, 261, 282-286.	3.1	47
27	Solid Hybrid Polymer Electrolyte Networks: Nano-Structurable Materials for Lithium Batteries. Advanced Materials, 2002, 14, 1134.	21.0	44
28	Crystal Structure and Sodium Environments in Sodium Tetratellurite, Na ₂ Te ₄ O ₉ , and Sodium Tellurite, Na ₂ TeO ₃ , by X-ray Crystallography and Sodium-23 NMR. Chemistry of Materials, 1994, 6, 1884-1889.	6.7	43
29	On the Formation of Tetracoordinate Boron in Rubidium Borate Glasses. Journal of the American Chemical Society, 1995, 117, 1397-1402.	13.7	43
30	Crystal Structures of Potassium Tetratellurite, K ₂ Te ₄ O ₉ , and Potassium Ditellurite, K ₂ Te ₂ O ₅ , and Structural Trends in Solid Alkali Tellurites. Inorganic Chemistry, 1997, 36, 5559-5564.	4.0	42
31	Structural aspects of the photoelastic response in lead borate glasses. Journal of Non-Crystalline Solids, 2011, 357, 2120-2125.	3.1	42
32	Design and applications of an in situ electrochemical NMR cell. Journal of Magnetic Resonance, 2011, 208, 136-147.	2.1	41
33	Solid Polymer Single-Ion Conductors: Synthesis and Properties. Chemistry of Materials, 2006, 18, 708-715.	6.7	39
34	Off-angle correlation spectroscopy applied to spin-1/2 and quadrupolar nuclei. Solid State Nuclear Magnetic Resonance, 1999, 13, 245-254.	2.3	35
35	Structural and dynamic properties of Y ₂ Mo ₃ O ₁₂ . Journal of Non-Crystalline Solids, 2011, 357, 2120-2125.	3.2	34
36	Sodium distribution in sodium tellurite glasses probed with spin-echo NMR. Physical Review B, 1997, 56, 5243-5249.	3.2	33

#	ARTICLE	IF	CITATIONS
37	Structure and properties of NaPO ₃ •ZnO•Nb ₂ O ₅ •Al ₂ O ₃ glasses. Journal of Non-Crystalline Solids, 2012, 358, 1795-1805.	3.1	32
38	Powder second-harmonic generation study of (K ₂ O) ₁₅ (Nb ₂ O ₅) ₁₅ (TeO ₂) ₇₀ glass ceramic. Applied Physics Letters, 2004, 85, 938-939.	3.3	31
39	A Neutron Scattering and Nuclear Magnetic Resonance Study of the Structure of GeO ₂ •P ₂ O ₅ Glasses. Journal of Physical Chemistry B, 2006, 110, 20123-20128.	2.6	30
40	Density-operator theory of orbital magnetic susceptibility in periodic insulators. Physical Review B, 2011, 84, .	3.2	30
41	Short-Range Structure of TeO ₂ Glass. Journal of Physical Chemistry C, 2017, 121, 28117-28124.	3.1	30
42	Assignment of the vibronic level structure of trimeric copper (Cu ₃) ground state. The Journal of Physical Chemistry, 1986, 90, 3298-3301.	2.9	29
43	On the mechanical properties of lead borate glass. Journal of Non-Crystalline Solids, 2013, 381, 29-34.	3.1	29
44	Self-Assembled Gyroidal Mesoporous Polymer-Derived High Temperature Ceramic Monoliths. Chemistry of Materials, 2016, 28, 2131-2137.	6.7	29
45	Investigation of Sodium Distribution in Phosphate Glasses Using Spin-Echo ²³ Na NMR. Journal of Physical Chemistry B, 2000, 104, 1464-1472.	2.6	28
46	A New Solid-State Proton Conductor: The Salt Hydrate Based on Imidazolium and 12-Tungstophosphate. Journal of the American Chemical Society, 2021, 143, 13895-13907.	13.7	28
47	Structure and chemical modification in oxide glasses. International Reviews in Physical Chemistry, 1998, 17, 65-90.	2.3	27
48	Semiclassical quantization of a classical analog for the Jahn-Teller system. Journal of Chemical Physics, 1986, 85, 2089-2098.	3.0	26
49	Synthesis of Metal-Loaded Poly(aminohexyl)(aminopropyl)silsesquioxane Colloids and Their Self-Organization into Dendrites. Nano Letters, 2002, 2, 873-876.	9.1	26
50	The NMR response of boroxol rings: a density functional theory study. Solid State Nuclear Magnetic Resonance, 2005, 27, 5-9.	2.3	25
51	A Comparison of Strategies for Obtaining High-Resolution NMR Spectra of Quadrupolar Nuclei. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1996, 51, 321-329.	1.5	25
52	The heat capacities of thermomiotic ScF ₃ and ScF ₃ •YF ₃ solid solutions. Journal of Materials Science, 2015, 50, 3409-3415.	3.7	24
53	Zero stress-optic barium tellurite glass. Journal of Non-Crystalline Solids, 2007, 353, 1662-1664.	3.1	23
54	Intermediate-Range Order of Alkali Disilicate Glasses and Its Relation to the Devitrification Mechanism. Journal of Physical Chemistry C, 2008, 112, 6151-6159.	3.1	23

#	ARTICLE	IF	CITATIONS
55	Controlled Synthesis of Novel Metalated Poly(aminoethyl)-(aminopropyl)silsesquioxane Colloids. <i>Langmuir</i> , 2003, 19, 7071-7083.	3.5	22
56	Composition and Morphology Control in Ordered Mesostructured High-Temperature Ceramics from Block Copolymer Mesophases. <i>Macromolecular Chemistry and Physics</i> , 2007, 208, 2096-2108.	2.2	22
57	Structural Similarity on Multiple Length Scales and Its Relation to Devitrification Mechanism: A Solid-State NMR Study of Alkali Diborate Glasses and Crystals. <i>Journal of Physical Chemistry C</i> , 2009, 113, 20725-20732.	3.1	22
58	Optical Implications of Crystallite Symmetry and Structure in Potassium Niobate Tellurite Glass Ceramics. <i>Chemistry of Materials</i> , 2002, 14, 4422-4429.	6.7	21
59	Residual internal stress in partially crystallized photothermorefractive glass: Evaluation by nuclear magnetic resonance spectroscopy and first principles calculations. <i>Journal of Applied Physics</i> , 2006, 99, 083511.	2.5	21
60	Relationships between elastic anisotropy and thermal expansion in $A_{2}Mo_{3}O_{12}$ materials. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30652-30661.	2.8	21
61	Crystal Structure of Sodium Ditellurite, $Na_{4}Te_{4}O_{10}$. <i>Acta Chemica Scandinavica</i> , 1997, 51, 118-121.	0.7	21
62	Topological constraints and the Makishima-Mackenzie model. <i>Journal of Non-Crystalline Solids</i> , 2015, 429, 20-23.	3.1	19
63	The Structure of GeS_{2} - $P_{2}S_{5}$ Glasses. <i>Journal of Physical Chemistry B</i> , 2002, 106, 11093-11101.	2.6	18
64	First-Principles Calculation of Electric Field Gradients in Metals, Semiconductors, and Insulators. <i>Applied Magnetic Resonance</i> , 2008, 33, 447-456.	1.2	18
65	The influence of intermetallic ordering on wear and indentation properties of TiC-Ni ₃ Al cermets. <i>Wear</i> , 2019, 426-427, 390-400.	3.1	18
66	On the Spectral Similarity of Bridging and Nonbridging Oxygen in Tellurites. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7636-7641.	2.5	17
67	Compositional dependence of the stress-optic response in zinc tellurite glasses. <i>Journal of Non-Crystalline Solids</i> , 2013, 381, 48-53.	3.1	17
68	Correlation of network structure with devitrification mechanism in lithium and sodium diborate glasses. <i>Journal of Non-Crystalline Solids</i> , 2010, 356, 2641-2644.	3.1	16
69	Finite homogeneous electric fields in the projector augmented wave formalism: Applications to linear and nonlinear response. <i>Computational Materials Science</i> , 2012, 58, 113-118.	3.0	16
70	Zero stress-optic bismuth oxide-based glass. <i>Journal of Non-Crystalline Solids</i> , 2018, 479, 82-89.	3.1	16
71	The glass forming ability of tellurites: a rigid polytope approach. <i>Journal of Non-Crystalline Solids</i> , 2003, 316, 273-280.	3.1	15
72	Correlation of Structure and Photoelastic Response in Tin Phosphate Glass. <i>International Journal of Applied Glass Science</i> , 2011, 2, 282-289.	2.0	15

#	ARTICLE	IF	CITATIONS
73	Relating ¹³⁹ La Quadrupolar Coupling Constants to Polyhedral Distortion in Crystalline Structures. <i>Journal of Physical Chemistry C</i> , 2015, 119, 25508-25517.	3.1	15
74	Structure and Ionic Interactions of Organic-Inorganic Composite Polymer Electrolytes Studied by Solid-State NMR and Raman Spectroscopy. <i>Solid State Nuclear Magnetic Resonance</i> , 2002, 22, 235-246.	2.3	14
75	¹²⁵ Te NMR Probes of Tellurium Oxide Crystals: Shielding-Structure Correlations. <i>Inorganic Chemistry</i> , 2018, 57, 892-898.	4.0	14
76	The Czjzek distribution in solid-state NMR: Scaling properties of central and satellite transitions. <i>Journal of Non-Crystalline Solids</i> , 2020, 550, 120383.	3.1	14
77	Stress, strain, and NMR. <i>Solid State Nuclear Magnetic Resonance</i> , 2006, 29, 113-118.	2.3	13
78	Computation of Mössbauer isomer shifts from first principles. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 195501.	1.8	13
79	Understanding the elastic and thermal response in TiC-based ceramic-metal composite systems: First-principles and mechanical studies. <i>Journal of Alloys and Compounds</i> , 2019, 789, 712-719.	5.5	13
80	Non-adiabatic rapid passage. <i>Chemical Physics Letters</i> , 2003, 375, 429-434.	2.6	12
81	Dependence of Conductivity on the Interplay of Structure and Polymer Dynamics in a Composite Polymer Electrolyte. <i>Journal of Physical Chemistry B</i> , 2004, 108, 918-928.	2.6	12
82	Observable effects of mechanical stress induced by sample spinning in solid state nuclear magnetic resonance. <i>Journal of Chemical Physics</i> , 2008, 128, 052304.	3.0	12
83	Structure and dynamics of ³ sE TM cyclopropane: A very fluxional multimode Jahn-Teller system. <i>Journal of Chemical Physics</i> , 1988, 89, 4012-4022.	3.0	11
84	Nanoindentation Study of the Surface of Ion-Exchanged Lithium Silicate Glass. <i>Journal of Physical Chemistry C</i> , 2016, 120, 5585-5598.	3.1	11
85	Amorphous orientation and its relationship to processing stages of blended polypropylene/polyethylene fibers. <i>Journal of Applied Polymer Science</i> , 2008, 108, 4047-4057.	2.6	10
86	First-principles study of the nuclear quadrupole resonance parameters and orbital ordering in LaTiO_3 . <i>Physical Review B</i> , 2009, 79, .	3.2	10
87	Elasto-Optic Coefficients of Borate, Phosphate, and Silicate Glasses: Determination by Brillouin Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2016, 120, 21802-21810.	3.1	10
88	Designing glass with non-dispersive stress-optic response. <i>Journal of Non-Crystalline Solids</i> , 2016, 433, 82-86.	3.1	10
89	Structural Differences between the Glass and Crystal Forms of the Transparent Ferroelectric Nanocomposite, LaBGeO_5 , from Neutron Diffraction and NMR Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2018, 122, 20963-20980.	3.1	10
90	Structural Study of Inorganic Oxides in a Hybrid Organic-Inorganic Solid Polymer Electrolyte. <i>Journal of Physical Chemistry B</i> , 2004, 108, 5851-5858.	2.6	9

#	ARTICLE	IF	CITATIONS
91	A ^{43}Ca and ^{13}C NMR study of the chemical interaction between poly(ethylene vinyl acetate) and white cement during hydration. <i>Solid State Nuclear Magnetic Resonance</i> , 2011, 40, 78-83.	2.3	9
92	The crystalline phase of $(\text{K}_2\text{O})_{15}(\text{Nb}_2\text{O}_5)_{15}(\text{TeO}_2)_7\text{O}$ glass ceramic is a polymorph of $\text{K}_2\text{Te}_4\text{O}_9$. <i>Journal of Non-Crystalline Solids</i> , 2004, 337, 48-53.	3.1	8
93	Glass-former/glass-modifier interactions and the stress-optic response. <i>Journal of Non-Crystalline Solids</i> , 2008, 354, 79-83.	3.1	8
94	Multinuclear NMR Study of Zinc Dicyanide. <i>Zeitschrift Fur Physikalische Chemie</i> , 2012, 226, 1205-1218.	2.8	8
95	Network Connectivity and Crystallization in the Transparent Ferroelectric Nanocomposite LaBGeO_5 . <i>Journal of Physical Chemistry C</i> , 2019, 123, 11860-11873.	3.1	8
96	The Relative Thermodynamic Stability of Diamond and Graphite. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 1546-1549.	13.8	8
97	Structure and properties of $\text{Ge}_{2.5}\text{PS}_x$ glasses. <i>Journal of Non-Crystalline Solids</i> , 2004, 333, 28-36.	3.1	7
98	Generalized Routes to Mesostructured Silicates with High Metal Content. <i>Zeitschrift Fur Physikalische Chemie</i> , 2012, 226, 1219-1228.	2.8	6
99	Elastic properties of ternary $(\text{Al}_x\text{Mg}_{1-x})\text{Sc}$ random alloys from first principles methods. <i>Journal of Alloys and Compounds</i> , 2014, 610, 138-142.	5.5	6
100	Quantization of a classical analog for the E \check{a} Š–e Jahn–Teller system at intermediate couplings. <i>Journal of Chemical Physics</i> , 1989, 90, 2357-2362.	3.0	5
101	Functional Polymer Colloids with Ordered Interior. <i>Langmuir</i> , 2004, 20, 1100-1110.	3.5	4
102	Correlating structure with stress-optic response in non-oxide glasses. <i>Journal of Non-Crystalline Solids</i> , 2014, 404, 1-6.	3.1	4
103	Computation of NMR observables: Consequences of projector-augmented wave sphere overlap. <i>Solid State Nuclear Magnetic Resonance</i> , 2016, 80, 14-18.	2.3	4
104	^{17}O NMR Spectroscopy of TeO_2 and Na_2TeO_3 . <i>Journal of the American Ceramic Society</i> , 2005, 88, 2325-2327.	3.8	3
105	Anisotropic stress in laser-written LaBGeO_5 glass-ceramic composites. <i>Journal of Applied Physics</i> , 2018, 124, .	2.5	2
106	Nuclear Magnetic Resonance and Electron Paramagnetic Resonance Studies of Glass. Springer Handbooks, 2019, , 955-995.	0.6	2
107	Intermediate Range Order in Sodium Tellurite Glasses. <i>Materials Research Society Symposia Proceedings</i> , 1996, 455, 405.	0.1	0
108	Borate Glass Structure Probed with Dynamic Angle Spinning NMR. <i>ACS Symposium Series</i> , 1999, , 242-255.	0.5	0

#	ARTICLE	IF	CITATIONS
109	The Structure of GeS ₂ -P ₂ S ₅ Glasses.. ChemInform, 2003, 34, no.	0.0	0
110	Spectral Similarity of Bridging and Nonbridging Oxygen in Tellurites.. ChemInform, 2005, 36, no.	0.0	0
111	Tuning the creep rates of binary Al alloys by considering the effects of the stacking faults, alloying elements, and elastic moduli: a first-principles study. Canadian Journal of Chemistry, 2018, 96, 755-759.	1.1	0
112	Solid-state nuclear magnetic resonance investigation of synthetic phlogopite and lepidolite samples. Magnetic Resonance in Chemistry, 2020, 58, 1099-1108.	1.9	0
113	The Relative Thermodynamic Stability of Diamond and Graphite. Angewandte Chemie, 2021, 133, 1570-1573.	2.0	0
114	New Information on the Structure and Dynamics of Molecular Cations from Experiments on The Spectroscopy of Polyatomic Rydberg States. , 1988, , 293-307.		0
115	High Resolution and Multidimensional Nuclear Magnetic Resonance Probes of Glass Structure. , 1997, , 245-254.		0