List of Publications by Year in descending order

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IOHN KIEFEED

#	Article	IF	CITATIONS
1	Mechanical degradation and viscous dissipation inB2O3. Physical Review B, 1994, 50, 17-29.	3.2	436
2	Lithium Ion Conducting Poly(ethylene oxide)-Based Solid Electrolytes Containing Active or Passive Ceramic Nanoparticles. Journal of Physical Chemistry C, 2017, 121, 2563-2573.	3.1	222
3	Energy Level Modulation of HOMO, LUMO, and Bandâ€Gap in Conjugated Polymers for Organic Photovoltaic Applications. Advanced Functional Materials, 2013, 23, 439-445.	14.9	152
4	Organic Dye Design Tools for Efficient Photocurrent Generation in Dyeâ€5ensitized Solar Cells: Exciton Binding Energy and Electron Acceptors. Advanced Functional Materials, 2012, 22, 1606-1612.	14.9	143
5	Amorphous-amorphous transitions in silica glass. I. Reversible transitions and thermomechanical anomalies. Physical Review B, 2004, 69, .	3.2	138
6	Flame made nanoparticles permit processing of dense, flexible, Li <sup>+</sup> conducting ceramic electrolyte thin films of cubic-Li <sub>7</sub> La <sub>3</sub> Zr <sub>2</sub> O <sub>12</sub> (c-LLZO). Journal of Materials Chemistry A, 2016, 4, 12947-12954.	10.3	131
7	Fluoreneâ€Based Oligomers for Highly Efficient and Stable Organic Blueâ€Lightâ€Emitting Diodes. Advanced Materials, 2009, 21, 2425-2429.	21.0	106
8	Amorphous-amorphous transitions in silica glass. II. Irreversible transitions and densification limit. Physical Review B, 2004, 69, .	3.2	99
9	Molecular dynamics study of cristobalite silica using a charge transfer three-body potential: Phase transformation and structural disorder. Journal of Chemical Physics, 2003, 118, 1487-1498.	3.0	96
10	Achieving Highly Efficient Fluorescent Blue Organic Lightâ€Emitting Diodes Through Optimizing Molecular Structures and Device Configuration. Advanced Functional Materials, 2011, 21, 699-707.	14.9	96
11	Structural transitions in silica glass: thermo-mechanical anomalies and polyamorphism. Journal of Non-Crystalline Solids, 2004, 349, 1-9.	3.1	80
12	Thermomechanical anomalies and polyamorphism inB2O3glass: A molecular dynamics simulation study. Physical Review B, 2006, 74, .	3.2	67
13	Design principles for the energy level tuning in donor/acceptor conjugated polymers. Physical Chemistry Chemical Physics, 2019, 21, 789-799.	2.8	63
14	Extended structural integrity in network glasses and liquids. Journal of Non-Crystalline Solids, 1997, 222, 190-198.	3.1	55
15	The role of curing stresses in subsequent response, damage and failure of textile polymer composites. Journal of the Mechanics and Physics of Solids, 2013, 61, 1241-1264.	4.8	55
16	Continuum and Molecular-Level Modeling of Fatigue Crack Retardation in Self-Healing Polymers. Journal of Engineering Materials and Technology, Transactions of the ASME, 2006, 128, 595-602.	1.4	54
17	The influence of the representative volume element (RVE) size on the homogenized response of cured fiber composites. Modelling and Simulation in Materials Science and Engineering, 2012, 20, 075007.	2.0	54
18	Materials that can replace liquid electrolytes in Li batteries: Superionic conductivities in Li1.7Al0.3Ti1.7Si0.4P2.6O12. Processing combustion synthesized nanopowders to free standing thin films. Journal of Power Sources, 2014, 269, 577-588.	7.8	53

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19	Thermal Conductance in Cross-linked Polymers: Effects of Non-Bonding Interactions. Journal of Physical Chemistry B, 2017, 121, 4600-4609.	2.6	50
20	Generation of heat and stress during the cure of polymers used in fiber composites. International Journal of Engineering Science, 2012, 53, 85-111.	5.0	48
21	Tuning Electronic Properties of Functionalized Polyhedral Oligomeric Silsesquioxanes: A DFT and TDDFT Study. Journal of Physical Chemistry A, 2009, 113, 9707-9714.	2.5	46
22	Charge Transfer as the Key Parameter Affecting the Color Purity of Thermally Activated Delayed Fluorescence Emitters. ACS Applied Materials & amp; Interfaces, 2021, 13, 28529-28537.	8.0	43
23	Origins of thermal boundary conductance of interfaces involving organic semiconductors. Journal of Applied Physics, 2012, 112, .	2.5	41
24	Molecular Dynamics Simulation Study of Growth Regimes during Polycondensation of Silicic Acid: from Silica Nanoparticles to Porous Gels. Journal of Physical Chemistry C, 2008, 112, 1764-1771.	3.1	40
25	Brillouin Light Scattering Investigation of the Mechanical Properties of Layer-by-Layer Assembled Cellulose Nanocrystal Films. Macromolecules, 2010, 43, 9541-9548.	4.8	34
26	<i>In Situ</i> Analysis of the Relationship between Cure Kinetics and the Mechanical Modulus of an Epoxy Resin. Macromolecules, 2014, 47, 8368-8376.	4.8	33
27	Structural developments in supercooled alkali tellurite melts. Physical Review B, 1998, 58, 694-705.	3.2	29
28	Ce-Substituted Nanograin Na <sub>3</sub> Zr <sub>2</sub> Si <sub>2</sub> PO <sub>12</sub> Prepared by LF-FSP as Sodium-Ion Conductors. ACS Applied Materials & Interfaces, 2020, 12, 3502-3509.	8.0	29
29	Molecular dynamic simulations of the infrared dielectric response of silica structures. Journal of Chemical Physics, 1993, 98, 8978-8986.	3.0	28
30	The complex mechanical modulus as a structural probe: The case of alkali borate liquids and glasses. Journal of Chemical Physics, 1995, 103, 9907-9917.	3.0	27
31	New Interpretation of Na <sup>+</sup> -lon Conduction in and the Structures and Properties of Sodium Borosilicate Mixed Glass Former Glasses. Journal of Physical Chemistry C, 2019, 123, 5853-5870.	3.1	27
32	Conjugated Copolymers That Shouldn't Be. Angewandte Chemie - International Edition, 2021, 60, 11115-11119.	13.8	25
33	Structural Relaxations in Alkali Silicate Systems by Brillouin Light Scattering. Journal of the American Ceramic Society, 1993, 76, 3073-3080.	3.8	24
34	High-frequency relaxational spectroscopy in liquid borates and silicates. Journal of Non-Crystalline Solids, 1995, 183, 51-60.	3.1	23
35	Molecular dynamic simulations of the α-β phase transition in silica cristobalite. Journal of Physics and Chemistry of Solids, 1998, 59, 1025-1037.	4.0	23
36	A new model linking elastic properties and ionic conductivity of mixed network former glasses. Physical Chemistry Chemical Physics, 2018, 20, 1629-1641.	2.8	23

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37	Temperature Dependence of the Highâ€Frequency Viscoelastic Behavior of a Sodaâ€Limeâ€&ilica Glass. Journal of the American Ceramic Society, 1998, 81, 1278-1284.	3.8	20
38	Effect of axial halogen substitution on the performance of subphthalocyanine based organic photovoltaic cells. Organic Electronics, 2014, 15, 3660-3665.	2.6	19
39	Anomalous thermomechanical properties and laser-induced densification of vitreous silica. Applied Physics Letters, 2006, 89, 141915.	3.3	18
40	Why do the [PhSiO <sub>1.5</sub> ] <sub>8,10,12</sub> cages self-brominate primarily in the ortho position? Modeling reveals a strong cage influence on the mechanism. Physical Chemistry Chemical Physics, 2014, 16, 25760-25764.	2.8	18
41	New Hybrid Method for the Calculation of the Solvation Free Energy of Small Molecules in Aqueous Solutions. Journal of Chemical Theory and Computation, 2019, 15, 371-381.	5.3	14
42	Unconventional Conjugation via vinylMeSi(Oâ^') <sub>2</sub> Siloxane Bridges May Imbue Semiconducting Properties in [vinyl(Me)SiO(PhSiO <sub>1.5</sub> ) <sub>8</sub> OSi(Me)vinyl-Ar] Double-Decker Copolymers. ACS Applied Polymer Materials, 2020, 2, 3894-3907.	4.4	13
43	Structural Transitions and Glass Formation. Journal of Physical Chemistry B, 1999, 103, 4153-4158.	2.6	12
44	Structural transitions and polyamorphism in glass-forming oxides. Journal of Non-Crystalline Solids, 2002, 307-310, 644-653.	3.1	12
45	Spatial nonuniformity in heat transport across hybrid material interfaces. Physical Review B, 2014, 90,	3.2	12
46	Elastic properties and short-range structural order in mixed network former glasses. Physical Chemistry Chemical Physics, 2017, 19, 15942-15952.	2.8	12
47	On the interplay between matter transport and structure formation at epoxy–hardener interfaces visualized by scanning Brillouin microscopy. Soft Matter, 2011, 7, 118-124.	2.7	11
48	Molecular Design Approach Managing Molecular Orbital Superposition for High Efficiency without Color Shift in Thermally Activated Delayed Fluorescent Organic Lightâ€Emitting Diodes. Chemistry - A European Journal, 2019, 25, 1829-1834.	3.3	11
49	Synthesis and Characterization of Nanobuilding Blocks [ <i>o-</i> RStyrPhSiO <sub>1.5</sub> ] <sub>10,12</sub> (R = Me, MeO, NBoc, and CN). Unexpected Photophysical Properties Arising from Apparent Asymmetric Cage Functionalization as Supported by Modeling Studies, Journal of Physical Chemistry C, 2015, 119, 15846-15858.	3.1	10
50	First Principles Study of Polymer-Metal—Metal-Oxide Adhesion. Journal of Adhesion, 1993, 42, 55-63.	3.0	9
51	Alkane–Metal Interfacial Structure and Elastic Properties by Molecular Dynamics Simulation. ACS Applied Materials & Interfaces, 2016, 8, 16885-16896.	8.0	9
52	Semiclassical model for calculating exciton and polaron pair energetics at interfaces. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2020, 261, 114657.	3.5	9
53	Fast relaxations in mixed-alkali silicates. Journal of Non-Crystalline Solids, 1999, 255, 56-66.	3.1	7
54	Spatially resolved, in situ elastic modulus of thermoset polymer amidst carbon fibers in a polymer matrix composite. Composites Science and Technology, 2014, 98, 22-27.	7.8	7

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55	Analysis of organic multilayered samples for optoelectronic devices by (lowâ€energy) dynamic SIMS. Surface and Interface Analysis, 2011, 43, 194-197.	1.8	6
56	Analysis and fragmentation of organic samples by (low-energy) dynamic SIMS. Surface and Interface Analysis, 2011, 43, 88-91.	1.8	6
57	Challenges in Modeling Mixed Ionic-Covalent Glass Formers. Springer Series in Materials Science, 2015, , 87-112.	0.6	6
58	Investigation of the transitional pore structure of activated carbon fibers by smallâ€angle neutron scattering. Journal of Applied Physics, 1992, 72, 5649-5656.	2.5	5
59	Silver Diffusion in Organic Optoelectronic Devices: Deposition-Related Processes versus Secondary Ion Mass Spectrometry Analysis Artifacts. Journal of Physical Chemistry C, 2015, 119, 23334-23341.	3.1	5
60	Predictive Simulations for Tuning Electronic and Optical Properties of SubPc Derivatives. Journal of Electronic Materials, 2019, 48, 2962-2970.	2.2	5
61	Magnetic anisotropy energies of M–Fe wires (M = V–Co) on vicinal Cu(111). RSC Advances, 2016, 6, 108948-108954.	3.6	4
62	Spectral mode assignment for binary silicate glasses using molecular dynamics simulations. Journal of Non-Crystalline Solids, 2012, 358, 3348-3354.	3.1	3
63	Substrate-Controlled Magnetism: Fe Nanowires on Vicinal Cu Surfaces. Nanomaterials, 2020, 10, 159.	4.1	3
64	Amplifying the Sensitivity of Polydiacetylene Sensors: The Dummy Molecule Approach. ACS Applied Materials & Interfaces, 2022, 14, 14561-14567.	8.0	3
65	Phase stability limits via non-equilibrium normal mode analysis. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1998, 77, 907-924.	0.6	2
66	Sputtering of silicon by lowâ€energy oxygen bombardment studied by MD simulations. Surface and Interface Analysis, 2013, 45, 356-359.	1.8	2
67	The role of halogen bonding in metal free phosphors. Physical Chemistry Chemical Physics, 2021, 23, 23351-23359.	2.8	2
68	Structural Relaxations in the GHz Frequency Range in Glass Forming Silicate Melts. Materials Research Society Symposia Proceedings, 1991, 248, 505.	0.1	1
69	Structural Developments in Fragile Glass Forming Oxides. Materials Research Society Symposia Proceedings, 1995, 407, 209.	0.1	1
70	Spac-Ttme-Correlations for Cation Motion in Alkali Silicates. Materials Research Society Symposia Proceedings, 1996, 455, 331.	0.1	1
71	MATERIALS SCIENCE: Not Too Hot to Handle. Science, 2003, 299, 1998-1999.	12.6	1
72	Fragility and the rate of change of the energy landscape topography. Journal of Non-Crystalline Solids: X, 2022, 14, 100101.	1.2	1

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73	Clustering and Extended Range Order in Binary Network Glasses. Materials Research Society Symposia Proceedings, 1995, 408, 363.	0.1	0
74	lonâ€matter interactions by MD simulations making use of reactive force fields. Surface and Interface Analysis, 2011, 43, 112-115.	1.8	0
75	Conjugated Copolymers That Shouldn't Be. Angewandte Chemie, 2021, 133, 11215-11219.	2.0	0
76	Anomalous Thermomechanical Properties of Network Glasses. Ceramic Engineering and Science Proceedings, 0, , 81-96.	0.1	0