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List of Publications by Year in descending order

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48
papers

780
citations

567144

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552653

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48
all docs

48
docs citations

48
times ranked

1099
citing authors

#	ARTICLE	IF	CITATIONS
1	Thermal conductivity of amorphous SiO ₂ by first-principles molecular dynamics. Journal of Non-Crystalline Solids, 2022, 581, 121434.	1.5	10
2	Structural, dynamical, and electronic properties of the ionic liquid 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide. Physical Chemistry Chemical Physics, 2022, 24, 9597-9607.	1.3	3
3	Atomic structure of amorphous SiN: Combining Car Parrinello and Born Oppenheimer first-principles molecular dynamics. Computational Materials Science, 2022, 211, 111555.	1.4	3
4	First-principles thermal transport in amorphous Ge ₂ Sb ₂ Te ₅ at the nanoscale. RSC Advances, 2021, 11, 10747-10752.	1.7	6
5	Quantitative assessment of the structure of amorphous Ge ₂₀ Se ₇ chalcogenide glass by first-principles molecular dynamics. Physical Review B, 2021, 103, .	1.1	4
6	Tridentate complexes of group 4 bearing bis-aryloxy N-heterocyclic carbene ligand: Structure, spin density and charge states. Chemical Physics Letters, 2021, 781, 138888.	1.2	0
7	Chalcogenide glasses for innovation in applied science: fundamental issues and new insights. Journal Physics D: Applied Physics, 2020, 53, 033002.	1.3	4
8	Thermal resistance of an interfacial molecular layer by first-principles molecular dynamics. Journal of Chemical Physics, 2020, 153, 074704.	1.2	7
9	Atomic Structure of Glassy GeTe ₄ as a Playground to Assess the Performances of Density Functional Schemes Accounting for Dispersion Forces. Journal of Physical Chemistry B, 2020, 124, 11273-11279.	1.2	7
10	Heat transport in disordered network forming materials: Size effects and existence of propagative modes. Computational Materials Science, 2020, 177, 109607.	1.4	4
11	Making Computer Materials Real: The Predictive Power of First-Principles Molecular Dynamics. Springer Series in Materials Science, 2020, , 3-21.	0.4	1
12	Assessing the Versatility of Molecular Modelling as a Strategy for Predicting Gas Adsorption Properties of Chalcogels. Springer Series in Materials Science, 2020, , 23-37.	0.4	0
13	Chalcogenide glasses as a playground for the application of first-principles molecular dynamics to disordered materials. Solid State Sciences, 2019, 95, 105925.	1.5	4
14	Thermal conductivity and transport modes in glassy GeTe ₄ by first-principles molecular dynamics. Physical Review Materials, 2019, 3, .	1.1	1
15	First-principles study of the atomic structure of glassy Ga ₁₀ Ge ₁₅ Te ₇₅ . Journal of Non-Crystalline Solids, 2018, 498, 338-344.	1.5	8
16	Organo-modified bentonite for gentamicin topical application: Interlayer structure and in vivo skin permeation. Applied Clay Science, 2018, 158, 158-168.	2.6	20
17	Sensitivity to Dispersion Forces in First-Principles Modeling of Disordered Chalcogenides. Frontiers in Materials, 2018, 5, .	1.2	7
18	On the occurrence of size effects in the calculation of thermal conductivity by first-principles molecular dynamics: The case of glassy GeTe ₄ . Journal of Non-Crystalline Solids, 2018, 498, 190-193.	1.5	13

#	ARTICLE	IF	CITATIONS
19	The structure and dipolar properties of CO ₂ adsorbed in a porous glassy chalcogel: Insights from first-principles molecular dynamics. Journal of Non-Crystalline Solids, 2018, 498, 288-293.	1.5	4
20	The role of dispersion forces on the atomic structure of glassy chalcogenides: The case of GeSe ₄ and GeS ₄ . Journal of Non-Crystalline Solids, 2018, 499, 167-172.	1.5	8
21	Evaluating the Critical Roles of Precursor Nature and Water Content When Tailoring Magnetic Nanoparticles for Specific Applications. ACS Applied Nano Materials, 2018, 1, 4306-4316.	2.4	22
22	First-Principles Study of Dissociation Processes for the Synthesis of Fe and Co Oxide Nanoparticles. Journal of Chemical Theory and Computation, 2018, 14, 225-235.	2.3	6
23	Thermal conductivity of glassy GeTe ₄ by first-principles molecular dynamics. Physical Chemistry Chemical Physics, 2017, 19, 9729-9732.	1.3	30
24	Layered Simple Hydroxides Functionalized by Fluorene-Phosphonic Acids: Synthesis, Interface Theoretical Insights, and Magnetoelectric Effect. Advanced Functional Materials, 2017, 27, 1703576.	7.8	20
25	Cooperative and Reversible Anisotropic Assembly of Gold Nanoparticles by Modulation of Noncovalent Interparticle Interactions. ChemNanoMat, 2017, 3, 874-878.	1.5	12
26	Impact of dispersion forces on the atomic structure of a prototypical network-forming disordered system: The case of liquid GeSe ₂ . Journal of Chemical Physics, 2017, 147, 044504.	1.2	9
27	Atomic-scale structure of the glassy GeSe_2 phase change material: A quantitative assessment via first-principles molecular dynamics. Physical Review B, 2017, 96, .	1.1	24
28	The role of 2D/3D spin-polarization interactions in hybrid copper hydroxide acetate: new insights from first-principles molecular dynamics. Beilstein Journal of Nanotechnology, 2017, 8, 857-860.	1.5	4
29	Nanoporous chalcogenides for adsorption and gas separation. Physical Chemistry Chemical Physics, 2016, 18, 13449-13458.	1.3	11
30	Pressure-induced structural changes in the network-forming isostatic glass GeSe_4 : An investigation by neutron diffraction and first-principles molecular dynamics. Physical Review B, 2016, 93, .	1.1	24
31	Role of the van der Waals interactions and impact of the exchange-correlation functional in determining the structure of glassy GeTe_4 . Physical Review B, 2015, 92, .	1.1	43
32	Comparison of Precipitated Calcium Carbonate/Poly(lactic Acid) and Halloysite/Poly(lactic Acid) Nanocomposites. Journal of Nanomaterials, 2015, 2015, 1-11.	1.5	16
33	Molecular Modeling of Glassy Surfaces. Springer Series in Materials Science, 2015, , 345-365.	0.4	1
34	Structure and Dynamics of Ionic Liquids Confined in Amorphous Porous Chalcogenides. Langmuir, 2015, 31, 6742-6751.	1.6	32
35	Origin of structural analogies and differences between the atomic structures of GeSe ₄ and GeS ₄ glasses: A first principles study. Journal of Chemical Physics, 2015, 143, 034504.	1.2	35
36	First-Principles Modeling of Binary Chalcogenides: Recent Accomplishments and New Achievements. Springer Series in Materials Science, 2015, , 313-344.	0.4	3

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37	Molecular dynamics simulation of amorphous HfO ₂ for resistive RAM applications. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 065006.	0.8	49
38	Surface of glassyGeS ₂ : A model based on a first-principles approach. Physical Review B, 2014, 90, .	1.1	16
39	Ionic liquid confined in silica nanopores: molecular dynamics in the isobaric isothermal ensemble. Molecular Physics, 2014, 112, 1350-1361.	0.8	71
40	First-principles molecular dynamics study of glassy GeS ₂ : Atomic structure and bonding properties. Physical Review B, 2013, 88, .	1.1	33
41	Immobilization of monolayer protected lipophilic gold nanorods on a glass surface. Nanotechnology, 2012, 23, 055605.	1.3	8
42	Comprehensive physical modeling of forming and switching operations in HfO ₂ RRAM devices. , 2011, , .		44
43	Insight into the structure of vanadium containing glasses: A molecular dynamics study. Journal of Non-Crystalline Solids, 2011, 357, 2571-2579.	1.5	41
44	Click Chemistry for the Assembly of Gold Nanorods and Silver Nanoparticles. Chemistry - A European Journal, 2011, 17, 9052-9056.	1.7	25
45	Microstructural characterisation and electrical properties of multiwalled carbon nanotubes/glass-ceramic nanocomposites. Journal of Materials Chemistry, 2010, 20, 308-313.	6.7	11
46	Double phase transfer of gold nanorods for surface functionalization and entrapment into PEG-based nanocarriers. Chemical Communications, 2009, , 5874.	2.2	61
47	Bentonite-Based Organoclays as Innovative Flame Retardants Agents for SBS Copolymer. Journal of Nanoscience and Nanotechnology, 2008, 8, 6316-6324.	0.9	5
48	Flame retardant SBS/clay nanocomposites. , 0, , 360-382.		0