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List of Publications by Year in descending order

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42 papers	1,172 citations	471371 17 h-index	395590 33 g-index
44 all docs	44 docs citations	44 times ranked	1207 citing authors

#	Article	IF	Citations
1		1.4	3
2	Induced ferromagnetism on late transition metals adsorbed on Antimony Arsenide monolayer from First-Principles. Journal of Magnetism and Magnetic Materials, 2022, 545, 168658.	1.0	1
3	First-principles thermal transport in amorphous Ge₂Sb₂Te₅ at the nanoscale. RSC Advances, 2021, 11, 10747-10752.	1.7	6
4	Quantitative assessment of the structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ge</mml:mi><mml:mn>20</mml:mn></mml:msub><mml:mo>(</mml:mo><mml:msub><mml:mi mathvariant="normal">I</mml:mi><mml:mn>7</mml:mn></mml:msub></mml:mrow></mml:math> chalcohalide glass by first-principles molecular dynamics. Physical Review B, 2021, 103, .	1.1	4
5	Chalcogenide glasses for innovation in applied science: fundamental issues and new insights. Journal Physics D: Applied Physics, 2020, 53, 033002.	1.3	4
6	Short range order and network connectivity in amorphous AsTe₃: a first principles, machine learning, and XRD study. Physical Chemistry Chemical Physics, 2020, 22, 24895-24906.	1.3	5
7	Atomic Structure of Glassy GeTe₄ 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
8	An enhanced coreâ€“shell interatomic potential for Teâ€“O based oxides. Materials Research Express, 2020, 7, 015202.	0.8	2
9	Making Computer Materials Real: The Predictive Power of First-Principles Molecular Dynamics. Springer Series in Materials Science, 2020, , 3-21.	0.4	1
10	Exploring Defects in Semiconductor Materials Through Constant Fermi Level Ab-Initio Molecular Dynamics. Springer Series in Materials Science, 2020, , 39-55.	0.4	0
11	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
12	Reaction pathway of oxygen evolution on Pt(1â€¯1â€¯1) revealed through constant Fermi level molecular dynamics. Journal of Catalysis, 2019, 375, 135-139.	3.1	19
13	Defect Formation Energies of Interstitial C, Si, and Ge Impurities in Î² â€Ga 2 O 3. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1800633.	1.2	11
14	Oxide versus Nonoxide Cathode Materials for Aqueous Zn Batteries: An Insight into the Charge Storage Mechanism and Consequences Thereof. ACS Applied Materials & Interfaces, 2019, 11, 674-682.	4.0	199
15	First-principles study of the atomic structure of glassy Ga10Ge15Te75. Journal of Non-Crystalline Solids, 2018, 498, 338-344.	1.5	8
16	Atomic-Scale Simulation of Electrochemical Processes at Electrode/Water Interfaces under Referenced Bias Potential. Journal of Physical Chemistry Letters, 2018, 9, 1880-1884.	2.1	72
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 GeTe4. Journal of Non-Crystalline Solids, 2018, 498, 190-193.	1.5	13

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19	The structure and dipolar properties of CO2 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 GeSe4 and GeS4. 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	Organic Cathode for Aqueous Zn-Ion Batteries: Taming a Unique Phase Evolution toward Stable Electrochemical Cycling. Chemistry of Materials, 2018, 30, 3874-3881.	3.2	373
23	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
24	Thermal conductivity of glassy GeTe₄by first-principles molecular dynamics. Physical Chemistry Chemical Physics, 2017, 19, 9729-9732.	1.3	30
25	Redox Levels through Constant Fermi-Level ab Initio Molecular Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 1769-1777.	2.3	24
26	Identification of Semiconductor Defects through Constant-Fermi-Level AbÂInitio Molecular Dynamics: Application to GaAs. Physical Review Applied, 2017, 8, .	1.5	4
27	Impact of dispersion forces on the atomic structure of a prototypical network-forming disordered system: The case of liquid GeSe2. Journal of Chemical Physics, 2017, 147, 044504.	1.2	9
28	Electron trap states at InGaAs/oxide interfaces under inversion through constant Fermi-levelab initiomolecular dynamics. Journal of Physics Condensed Matter, 2017, 29, 505702.	0.7	4
29	Atomic-scale structure of the glassy <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ge</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> phase change material: A quantitative assessment via first-principles molecular dynamics. Physical Review B, 2017, 96, .	1.1	24
30	Structure of amorphous GeSe9 by neutron diffraction and first-principles molecular dynamics: Impact of trajectory sampling and size effects. Journal of Chemical Physics, 2016, 145, 084502.	1.2	6
31	Pressure-induced structural changes in the network-forming isostatic glass<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>GeSe</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math> An investigation by neutron diffraction and first-principles molecular dynamics. Physical Review B, 2016, 93, .	1.1	24
32	Role of the van der Waals interactions and impact of the exchange-correlation functional in determining the structure of glassyGeTe4. Physical Review B, 2015, 92, .	1.1	43
33	Molecular Modeling of Glassy Surfaces. Springer Series in Materials Science, 2015, , 345-365.	0.4	1
34	First-principles study of amorphous<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ga</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> alloys. Physical Review B, 2015, 91, .	1.1	21
35	Origin of structural analogies and differences between the atomic structures of GeSe4 and GeS4 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	Density-driven defect-mediated network collapse of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">GeSe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>glass. Physical Review B, 2014, 90, .	1.1	30
38	Surface of glassyGeS2: A model based on a first-principles approach. Physical Review B, 2014, 90, .	1.1	16
39	The structure of liquid GeSe revisited: A first principles molecular dynamics study. Journal of Chemical Physics, 2013, 138, 174505.	1.2	21
40	First-principles molecular dynamics study of glassy GeS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>: Atomic structure and bonding properties. Physical Review B, 2013, 88, .	1.1	33
41	Note: Accounting for pressure effects on the calculated equilibrium structure of glassy GeSe2. Journal of Chemical Physics, 2012, 137, 046101.	1.2	25
42	Structural properties of glassy Ge<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Se<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>from first-principles molecular dynamics. Physical Review B, 2012, 86, .	1.1	33