Sergey I Morozov

List of Publications by Year
in descending order

32 papers	599 citations	687363 13 h-index	610901 24 g-index
32 all docs	32 docs citations	32 times ranked	845 citing authors

#	Article	IF	Citations
1	Quantum Mechanics Reactive Dynamics Study of Solid Li-Electrode/Li₆PS₅Cl-Electrolyte Interface. ACS Energy Letters, 2017, 2, 1454-1459.	17.4	83
2	Ductile deformation mechanism in semiconductor Î±-Ag2S. Npj Computational Materials, 2018, 4, .	8.7	54
3	Superstrengthening <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Bi</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub><m through Nanotwinning. Physical Review Letters, 2017, 119, 085501.	7.8	53
4	Design of a Graphene Nitrene Two-Dimensional Catalyst Heterostructure Providing a Well-Defined Site Accommodating One to Three Metals, with Application to CO₂ Reduction Electrocatalysis for the Two-Metal Case. Journal of Physical Chemistry Letters, 2020, 11, 2541-2549.	4.6	51
5	Enhanced Strength Through Nanotwinning in the Thermoelectric Semiconductor InSb. Physical Review Letters, 2017, 119, 215503.	7.8	45
6	Mechanism and kinetics of the electrocatalytic reaction responsible for the high cost of hydrogen fuel cells. Physical Chemistry Chemical Physics, 2017, 19, 2666-2673.	2.8	43
7	Fracture toughness of thermoelectric materials. Materials Science and Engineering Reports, 2021, 144, 100607.	31.8	39
8	Interface Structure in Li-Metal/[Pyr₁₄][TFSI]-Ionic Liquid System from ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2019, 10, 4577-4586.	4.6	31
9	Dramatically reduced lattice thermal conductivity of Mg2Si thermoelectric material from nanotwinning. Acta Materialia, 2019, 169, 9-14.	7.9	30
10	Mechanical properties in thermoelectric oxides: Ideal strength, deformation mechanism, and fracture toughness. Acta Materialia, 2018, 149, 341-349.	7.9	25
11	Light irradiation induced brittle-to-ductile and ductile-to-brittle transition in inorganic semiconductors. Physical Review B, 2019, 99, .	3.2	16
12	First-Principles Modeling of Ni₄M (M = Co, Fe, and Mn) Alloys as Solid Oxide Fuel Cell Anode Catalyst for Methane Reforming. Journal of Physical Chemistry C, 2016, 120, 207-214.	3.1	15
13	Icosahedra clustering and short range order in Ni-Nb-Zr amorphous membranes. Scientific Reports, 2018, 8, 6084.	3.3	13
14	Mechanical softening of thermoelectric semiconductor Mg2Si from nanotwinning. Scripta Materialia, 2018, 157, 90-94.	5.2	13
15	Photomechanical effect leading to extraordinary ductility in covalent semiconductors. Physical Review B, 2019, 100, .	3.2	11
16	Grain Boundaries Softening Thermoelectric Oxide BiCuSeO. ACS Applied Materials & Interfaces, 2018, 10, 6772-6777.	8.0	10
17	Determining ideal strength and failure mechanism of thermoelectric CuInTe2 through quantum mechanics. Journal of Materials Chemistry A, 2018, 6, 11743-11750.	10.3	10
18	Nanotwin-induced ductile mechanism in thermoelectric semiconductor PbTe. Matter, 2022, 5, 1839-1852.	10.0	10

#	Article	IF	Citations
19	Li-diffusion at the interface between Li-metal and [Pyr14][TFSI]-ionic liquid: Ab initio molecular dynamics simulations. Journal of Chemical Physics, 2020, 152, 031101.	3.0	9
20	Brittle failure of Î²- and Ï„-boron: Amorphization under high pressure. Physical Review B, 2017, 95, .	3.2	8
21	Reduction of N₂ to Ammonia by Phosphate Molten Salt and Li Electrode: Proof of Concept Using Quantum Mechanics. Journal of Physical Chemistry Letters, 2021, 12, 1696-1701.	4.6	6
22	Intrinsic mechanical behavior of MgAgSb thermoelectric material: An ab initio study. Journal of Materiomics, 2020, 6, 24-32.	5.7	5
23	Estimating the lower-limit of fracture toughness from ideal-strength calculations. Materials Horizons, 2022, 9, 825-834.	12.2	4
24	The Mechanism of Deformation and Failure of In4Se3 Based Thermoelectric Materials. ACS Applied Energy Materials, 2020, 3, 1054-1062.	5.1	3
25	Characterizing local metallic bonding variation induced by external perturbation. Physical Chemistry Chemical Physics, 2020, 22, 2372-2378.	2.8	3
26	Reaction Mechanism and Energetics of Decomposition of Tetrakis(1,3-dimethyltetrazol-5-imidoperchloratomanganese(II)) from Quantum-Mechanics-based Reactive Dynamics. Journal of the American Chemical Society, 2021, 143, 16960-16975.	13.7	3
27	Li, An, and Morozov Reply:. Physical Review Letters, 2019, 123, 119602.	7.8	2
28	Enhancing the shear strength of single-crystalline In4Se3 through point defects. Scripta Materialia, 2022, 211, 114507.	5.2	2
29	Proton transport mechanism and pathways in the superprotonic phase of M3H(AO4)2 solid acids from ab initio molecular dynamics simulations. Physical Chemistry Chemical Physics, 2021, 23, 17026-17032.	2.8	1
30	Deformation and Failure Mechanisms of Thermoelectric Type-I Clathrate Ba₈Au₆Ge₄₀. ACS Applied Materials & Interfaces, 2022, 14, 4326-4334.	8.0	1
31	Application of modern software packages to calculating the solidification of high-speed steels. Russian Metallurgy (Metally), 2015, 2015, 962-963.	0.5	0
32	Atomistic explanation of failure mechanisms of thermoelectric type-VIII clathrate Ba8Ga16Sn30. Materials Today Communications, 2022, 31, 103605.	1.9	0