List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Structural characterization of deformed crystals by analysis of common atomic neighborhood. Computer Physics Communications, 2007, 177, 518-523.	7.5	567
2	Interaction potential forSiO2: A molecular-dynamics study of structural correlations. Physical Review B, 1990, 41, 12197-12209.	3.2	539
3	Interaction potential for silicon carbide: A molecular dynamics study of elastic constants and vibrational density of states for crystalline and amorphous silicon carbide. Journal of Applied Physics, 2007, 101, 103515.	2.5	283
4	Intermediate-range order in permanently densified vitreousSiO2: A neutron-diffraction and molecular-dynamics study. Physical Review B, 1991, 43, 1194-1197.	3.2	274
5	Structure of rings in vitreousSiO2. Physical Review B, 1993, 47, 3053-3062.	3.2	216
6	Molecular Dynamics Simulation of Structural Transformation in Silicon Carbide under Pressure. Physical Review Letters, 2000, 84, 3338-3341.	7.8	183
7	Interaction potentials for alumina and molecular dynamics simulations of amorphous and liquid alumina. Journal of Applied Physics, 2008, 103, .	2.5	139
8	90° domain wall relaxation and frequency dependence of the coercive field in the ferroelectric switching process. Journal of Applied Physics, 2004, 95, 2646-2653.	2.5	110
9	Structural transformation in densified silica glass: A molecular-dynamics study. Physical Review B, 1994, 50, 118-131.	3.2	107
10	Structural transformation, intermediate-range order, and dynamical behavior ofSiO2glass at high pressures. Physical Review Letters, 1993, 71, 3146-3149.	7.8	95
11	Structural and dynamical correlations in Ag2Se: A molecular dynamics study of superionic and molten phases. Journal of Chemical Physics, 1988, 89, 7542-7555.	3.0	80
12	Dynamic structure factor and vibrational properties ofSiO2glass. Physical Review B, 1993, 48, 9359-9368.	3.2	73
13	Short- and intermediate-range structural correlations in amorphous silicon carbide: A molecular dynamics study. Physical Review B, 2004, 70, .	3.2	65
14	Interaction potential for aluminum nitride: A molecular dynamics study of mechanical and thermal properties of crystalline and amorphous aluminum nitride. Journal of Applied Physics, 2011, 109, .	2.5	62
15	Atomistic damage mechanisms during hypervelocity projectile impact on AlN: A large-scale parallel molecular dynamics simulation study. Journal of the Mechanics and Physics of Solids, 2008, 56, 1955-1988.	4.8	50
16	Molecular dynamics simulation of fast dislocations in copper. Acta Materialia, 2009, 57, 1843-1855.	7.9	47
17	Accelerating dislocations to transonic and supersonic speeds in anisotropic metals. Applied Physics Letters, 2008, 92, .	3.3	40
18	Diffusivity, Interfacial Free Energy, and Crystal Nucleation in a Supercooled Lennard-Jones Liquid. Journal of Physical Chemistry C, 2018, 122, 28884-28894.	3.1	40

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19	Topology of amorphous gallium arsenide on intermediate length scales: A molecular dynamics study. Journal of Applied Physics, 2000, 87, 7708-7711.	2.5	34
20	Dynamic behaviour of silicon carbide nanowires under high and extreme strain rates: a molecular dynamics study. Journal Physics D: Applied Physics, 2011, 44, 055405.	2.8	33
21	Successful test of the classical nucleation theory by molecular dynamic simulations of BaS. Computational Materials Science, 2019, 161, 99-106.	3.0	30
22	Pressure-induced structural transformation in GaAs: A molecular-dynamics study. Physical Review B, 2002, 65, .	3.2	29
23	Molecular dynamics study of structural, mechanical, and vibrational properties of crystalline and amorphous Ga1â^'xInxAs alloys. Journal of Applied Physics, 2003, 94, 3840-3848.	2.5	28
24	Structural, mechanical, and vibrational properties of Ga1â~'xInxAs alloys: A molecular dynamics study. Applied Physics Letters, 2003, 82, 1057-1059.	3.3	27
25	Interaction potential for indium phosphide: a molecular dynamics and first-principles study of the elastic constants, generalized stacking fault and surface energies. Journal of Physics Condensed Matter, 2009, 21, 095002.	1.8	25
26	Energetics of phase transitions in BaO through DFT calculations with norm-conserving pseudopotentials: LDA vs. GGA results. Computational Materials Science, 2006, 37, 349-354.	3.0	24
27	Shock-induced microstructural response of mono- and nanocrystalline SiC ceramics. Journal of Applied Physics, 2018, 123, .	2.5	24
28	Crystal Nucleation Kinetics in Supercooled Germanium: MD Simulations versus Experimental Data. Journal of Physical Chemistry B, 2020, 124, 7979-7988.	2.6	23
29	Plane shock loading on mono- and nano-crystalline silicon carbide. Applied Physics Letters, 2018, 112, .	3.3	22
30	Tailoring Electronic Transparency of Twin-Plane 1D Superlattices. ACS Nano, 2011, 5, 5519-5525.	14.6	21
31	Structural phase transition and dynamical properties of PbTiO3simulated by molecular dynamics. Journal of Physics Condensed Matter, 2005, 17, 5771-5783.	1.8	20
32	Molecular dynamics simulations of spontaneous and seeded nucleation and theoretical calculations for zinc selenide. Computational Materials Science, 2021, 187, 110124.	3.0	19
33	Atomistic simulation of the deformation mechanism during nanoindentation of gamma titanium aluminide. Computational Materials Science, 2012, 62, 1-5.	3.0	17
34	High-pressure phases of InP: An ab initio and molecular-dynamics study. Applied Physics Letters, 2006, 88, 161919.	3.3	15
35	Structural and dynamic properties of vitreous and crystalline barium disilicate: molecular dynamics simulation and Raman scattering experiments. Journal Physics D: Applied Physics, 2016, 49, 435301.	2.8	14
36	Properties of surface electrons on a helium film: Effects of the film thickness and substrate. Physical Review B, 1984, 29, 2584-2588.	3.2	13

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37	Molecular dynamics simulation of the structural and dynamical properties of crystalline BaO. Physical Review B, 2005, 71, .	3.2	13
38	Structural phase transformation in InSb: $\hat{a} \in f A$ molecular dynamics simulation. Physical Review B, 2002, 66, $\cdot$	3.2	12
39	Molecular-dynamics prediction of the thermal conductivity of thin InP nanowires: Similarities to Si. Physical Review B, 2009, 80, .	3.2	12
40	Diffusion mechanisms in lithium disilicate melt by molecular dynamics simulation. Journal of Non-Crystalline Solids, 2014, 402, 91-95.	3.1	12
41	Melting of classical two-dimensional electrons on a helium film: A molecular-dynamics study. Physical Review B, 1996, 54, 7046-7051.	3.2	11
42	A dynamic pathway for the alkaline earth oxides B1 to B2 transformation. Europhysics Letters, 2006, 76, 836-841.	2.0	11
43	Interaction potential for ZnTe: A molecular dynamics study. Physical Review B, 2005, 72, .	3.2	10
44	Structural ordering in CdxPb1â^'xF2 alloys: A combined molecular dynamics and solid state NMR study. Journal of Chemical Physics, 2008, 128, 224705.	3.0	10
45	Nonlinear dielectric response and transient current: An effective potential for ferroelectric domain wall displacement. Applied Physics Letters, 2013, 103, .	3.3	10
46	Structural phase transformations in InP under pressure: A molecular-dynamics study. Physica Status Solidi (B): Basic Research, 2007, 244, 239-243.	1.5	9
47	Unveiling nucleation dynamics by seeded and spontaneous crystallization in supercooled liquids. Computational Materials Science, 2021, 199, 110802.	3.0	9
48	An interaction potential for barium sulfide: A molecular dynamics study. Computational Materials Science, 2014, 92, 334-342.	3.0	8
49	Unveiling relaxation and crystal nucleation interplay in supercooled germanium liquid. Acta Materialia, 2021, 220, 117303.	7.9	8
50	Molecular dynamics study of amorphous InSb. Journal of Non-Crystalline Solids, 2004, 348, 17-21.	3.1	7
51	Glass Forming Ability and Alloying Effect of a Noble-Metal-Based Glass Former. Journal of Physical Chemistry B, 2012, 116, 1356-1359.	2.6	6
52	The race between relaxation and nucleation in supercooled liquid and glassy BaS – A molecular dynamics study. Computational Materials Science, 2021, 192, 110417.	3.0	6
53	Relaxation, crystal nucleation, kinetic spinodal and Kauzmann temperature in supercooled zinc selenide. Computational Materials Science, 2021, 193, 110421.	3.0	6
54	Um potencial de interação para o estudo de materiais e simulações por dinâmica molecular. Quimica Nova, 2001, 24, 838-845.	0.3	5

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55	The eutectic composition on Cd x Pb 1 â^ x F 2 phase diagram: A molecular-dynamics study. Europhysics Letters, 2005, 71, 770-775.	2.0	5
56	Vibrational properties of InP under pressure: a molecular-dynamics study. Physica Status Solidi (B): Basic Research, 2007, 244, 331-335.	1.5	5
57	Low-temperature elastic anomalies in CaTiO <sub>3</sub> : dynamical characterization. Journal of Physics Condensed Matter, 2012, 24, 475401.	1.8	5
58	On the transferability of interaction potentials for condensed phases of silicon. Journal of Molecular Liquids, 2019, 285, 488-499.	4.9	5
59	Theory of electron transport in a two-dimensional layer on the solid hydrogen surface. Physical Review B, 1995, 51, 11068-11073.	3.2	4
60	Interaction potential for InSb: a molecular dynamics study. Brazilian Journal of Physics, 2004, 34, 347.	1.4	4
61	Molecular dynamics simulations on the local order of liquid and amorphous ZnTe. Journal of Chemical Physics, 2008, 128, 184704.	3.0	4
62	Temperature and Pinning Effects on Driving a 2D Electron System on a Helium Film: A Numerical Study. Journal of Low Temperature Physics, 2010, 160, 58-67.	1.4	4
63	Evidence for the formation of metallic In after laser irradiation of InP. Journal of Applied Physics, 2019, 126, .	2.5	4
64	Direct determination of Lennard-Jones crystal surface free energy by a computational cleavage method. Journal of Chemical Physics, 2021, 155, 094101.	3.0	4
65	Decoding crystal growth kinetics and structural evolution in supercooled ZnSe by molecular dynamics simulation. Computational Materials Science, 2022, 212, 111598.	3.0	4
66	Molecular dynamics simulation on devitrification: Isothermal devitrification and thermodynamics of PbF2 glasses. Journal of Chemical Physics, 2004, 121, 7413-7420.	3.0	3
67	An interatomic potential for aluminum arsenide: A molecular dynamics study. Computational Materials Science, 2010, 49, 270-275.	3.0	3
68	Ferroelectric Domain Wall as Stretched Membrane: Nonlinear Dielectric Response and Tunability. Ferroelectrics, 2014, 461, 29-37.	0.6	3
69	Domain wall contribution to the nonlinear dielectric response: effective potential model. Journal Physics D: Applied Physics, 2015, 48, 465301.	2.8	3
70	Finite size effects on a core-shell model of barium titanate. Computational Materials Science, 2017, 130, 98-102.	3.0	3
71	Charged-hard-sphere system: A self-consistent-field approximation. Physical Review E, 1993, 48, 1375-1378.	2.1	2
72	Insulator-conductor behavior of a two-dimensional electron system on a helium film. Physical Review B, 2008, 77, .	3.2	2

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73	On the use of atomistic simulations to aid bulk metallic glasses structural elucidation with solid-state NMR. Scientific Reports, 2017, 7, 9305.	3.3	2
74	Neural Network Quantum Molecular Dynamics, Intermediate Range Order in GeSe <sub>2</sub> , and Neutron Scattering Experiments. Journal of Physical Chemistry Letters, 2021, 12, 6020-6028.	4.6	2
75	The two-dimensional polystyrene spheres in the hypernetted chain approximation. Journal of Physics C: Solid State Physics, 1982, 15, L893-L898.	1.5	1
76	Simulation of the Polarization Switching in Ferroelectrics with Dipolar Defects Through the Landau-Theory-Based Lattice Model. Ferroelectrics, 2004, 300, 173-176.	0.6	1
77	Oscilações paramétricas: uma simulação numérica. Revista Brasileira De Ensino De Fisica, 2007, 29, 71-	7 <b>8.</b> 2	1
78	Reply to the Comment by I. I. Buchinskaya and P. P. Fedorov. Europhysics Letters, 2008, 83, 16002.	2.0	1
79	The structural inhomogeneity of lead–cadmium fluoride systems and its implications. Journal of Physics Condensed Matter, 2009, 21, 335107.	1.8	1
80	Crystallization kinetics of a 2D system using molecular dynamics simulation. Journal of Physics Condensed Matter, 2010, 22, 455106.	1.8	1
81	Tuning hole mobility in InP nanowires. Applied Physics Letters, 2012, 101, 182104.	3.3	1
82	An interaction potential for zinc selenide: A molecular dynamics study. Journal of Applied Physics, 2021, 129, .	2.5	1
83	Bragg Intensities and Diffuse Scattering in Ag2Se: A Molecular Dynamics Study. , 1991, , 171-187.		1
84	Interaction potentials for alumina and molecular dynamics simulations of amorphous and liquid alumina. , 0, .		1
85	Polarization Switching Relaxation in Pb(Zr,Ti)O3 Ceramics. Integrated Ferroelectrics, 2004, 62, 115-118.	0.7	0
86	Dynamical structure factor of two-dimensional electrons over a helium film. Low Temperature Physics, 2008, 34, 388-391.	0.6	0
87	Análise de um estilingue e espirais de caderno: um estudo de caso. Revista Brasileira De Ensino De Fisica, 2006, 28, 195-199.	0.2	0