Inna Ponomareva

List of Publications by Year
in descending order

68 papers	2,439 citations	257450 24 h-index	197818 49 g-index
68 all docs	68 docs citations	68 times ranked	2120 citing authors

#	Article	IF	Citations
1	Bridging the Macroscopic and Atomistic Descriptions of the Electrocaloric Effect. Physical Review Letters, 2012, 108, 167604.	7.8	209
2	Coexistence of the Phonon and Relaxation Soft Modes in the Terahertz Dielectric Response of Tetragonal<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2008, 101, 167402.	7.8	191
3	Thermal Conductivity in Thin Silicon Nanowires:Â Phonon Confinement Effect. Nano Letters, 2007, 7, 1155-1159.	9.1	170
4	Atomistic treatment of depolarizing energy and field in ferroelectric nanostructures. Physical Review B, 2005, 72, .	3.2	132
5	Terahertz dielectric response of cubic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Ba</mml:mi><mml:mi mathvariant="normal">Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2008, 77, .	3.2	125
6	Finite-temperature flexoelectricity in ferroelectric thin films from first principles. Physical Review B, 2012, 85, .	3.2	119
7	Electric-Field-Induced Domain Evolution in Ferroelectric Ultrathin Films. Physical Review Letters, 2006, 96, 137602.	7.8	107
8	Low-dimensional ferroelectrics under different electrical and mechanical boundary conditions: Atomistic simulations. Physical Review B, 2005, 72, .	3.2	101
9	Multicaloric effect in ferroelectric PbTiO<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. Physical Review B, 2013, 87, .	3.2	83
10	Electrocaloric effect in bulk and low-dimensional ferroelectrics from first principles. Physical Review B, 2008, 78, .	3.2	76
11	Control of Vortices by Homogeneous Fields in Asymmetric Ferroelectric and Ferromagnetic Rings. Physical Review Letters, 2008, 100, 047201.	7.8	76
12	Structure, Stability, and Quantum Conductivity of Small Diameter Silicon Nanowires. Physical Review Letters, 2005, 95, 265502.	7.8	67
13	Low-Symmetry Phases in Ferroelectric Nanowires. Nano Letters, 2010, 10, 1177-1183.	9.1	62
14	Giant elastocaloric effect in ferroelectric Ba<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>0.5</mml:mn></mml:mrow></mml:msub></mml:math>Sr<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>0.5</mml:mn></mml:mrow></mml:msub></mml:math>TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:	3.2	62
15	Intrinsic electrocaloric effect in ferroelectric alloys from atomistic simulations. Physical Review B, 2009, 80, .	3.2	50
16	Critical Thickness for Antiferroelectricity in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>PbZrO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn>< Physical Review Letters, 2015, 115, 097601.	7.8	48
17	Thickness dependency of 180Â° stripe domains in ferroelectric ultrathin films: A first-principles-based study. Applied Physics Letters, 2007, 91, .	3.3	45
18	Finite-temperature properties of antiferroelectric<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>PbZrO</mml:mi><mml:mn>3</mml:mn></mml:msub></m atomistic simulations. Physical Review B, 2015, 91, .	3.2	43

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19	Unusual static and dynamical characteristics of domain evolution in ferroelectric superlattices. Physical Review B, 2009, 79, .	3.2	34
20	Atomistic study of soft-mode dynamics in PbTiO<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>. Physical Review B, 2013, 88, .	3.2	34
21	Dielectric Anomalies in Ferroelectric Nanostructures. Physical Review Letters, 2007, 99, 227601.	7.8	32
22	Electrocaloric effect in ferroelectric nanowires from atomistic simulations. Scientific Reports, 2015, 5, 17294.	3.3	32
23	Influence of the growth direction on properties of ferroelectric ultrathin films. Physical Review B, 2006, 74, .	3.2	29
24	Nanodynamics of Ferroelectric Ultrathin Films. Physical Review Letters, 2011, 107, 177601.	7.8	27
25	Nature of Dynamical Coupling between Polarization and Strain in Nanoscale Ferroelectrics from First Principles. Physical Review Letters, 2008, 101, 197602.	7.8	25
26	Elastocaloric Effect in Carbon Nanotubes and Graphene. Nano Letters, 2016, 16, 7008-7012.	9.1	24
27	Tailoring properties of ferroelectric ultrathin films by partial charge compensation. Applied Physics Letters, 2014, 104, .	3.3	22
28	Microscopic Insight into Temperature-Graded Ferroelectrics. Physical Review Letters, 2010, 105, 147602.	7.8	21
29	Emergence of central mode in the paraelectric phase of ferroelectric perovskites. MRS Communications, 2013, 3, 41-45.	1.8	20
30	Thermally Mediated Mechanism to Enhance Magnetoelectric Coupling in Multiferroics. Physical Review Letters, 2015, 114, 177205.	7.8	20
31	Scaling law for electrocaloric temperature change in antiferroelectrics. Scientific Reports, 2016, 6, 19590.	3.3	20
32	Electrocaloric effect in PbZrO3 thin films with antiferroelectric-ferroelectric phase competition. Computational Materials Science, 2017, 129, 44-48.	3.0	20
33	Phase Switching as the Origin of Large Piezoelectric Response in Organic-Inorganic Perovskites: A First-Principles Study. Physical Review Letters, 2020, 125, 207601.	7.8	20
34	Dynamics of antiferroelectric phase transition in PbZrO3. Physical Review B, 2017, 96, .	3.2	20
35	Phase diagrams of epitaxial<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Pb</mml:mtext><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mtext>Zr</mml:mt films from first principles. Physical Review B, 2009, 80, .	3.2	19
36	Competing polarization reversal mechanisms in ferroelectric nanowires. Physical Review B, 2012, 86, .	3.2	17

#	ARTICLE	IF	CITATIONS
37	Advanced Photoemission Spectroscopy Investigations Correlated with DFT Calculations on the Self-Assembly of 2D Metal Organic Frameworks Nano Thin Films. ACS Applied Materials & Interfaces, 2016, 8, 31403-31412.	8.0	17
38	Infrared and THz Soft-Mode Spectroscopy of (Ba,Sr)TiO3 Ceramics. Ferroelectrics, 2008, 367, 139-148.	0.6	13
39	Diffuse phase transitions in ferroelectric ultrathin films from first principles. Physical Review B, 2010, 81, .	3.2	11
40	Highly tunable piezocaloric effect in antiferroelectric<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">PbZrO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2016, 93, .	3.2	11
41	Prediction of high-strain polar phases in antiferroelectric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>PbZrO</mml:mi><mml:mn>3</mml:mn></mml:msub></m from a multiscale approach. Physical Review B, 2020, 102, .	3.2	11
42	Tunability of Structure, Polarization, and Band Gap of High TC Organicâ€"Inorganic Ferroelectrics by Hydrostatic Pressure: First-Principles Study. Journal of Physical Chemistry C, 2021, 125, 16296-16303.	3.1	11
43	Lattice dynamics in Ba_{0.7}Sr_{0.3}TiO₃: study by THz and IR spectroscopy and<i>ab initio</i>simulations. Phase Transitions, 2010, 83, 955-965.	1.3	10
44	Terahertz sensing using ferroelectric nanowires. Nanotechnology, 2013, 24, 045501.	2.6	10
45	Emergence of ferroelectricity in antiferroelectric nanostructures. Nanotechnology, 2016, 27, 195705.	2.6	10
46	Depolarizing field in ultrathin electrocalorics. Physical Review B, 2015, 92, .	3.2	9
47	Unveiling Electrocaloric Potential of Antiferroelectrics with Phase Competition. Advanced Theory and Simulations, 2018, 1, 1800096.	2.8	9
48	High-frequency intrinsic dynamics of the electrocaloric effect from direct atomistic simulations. Physical Review B, 2018, 97, .	3.2	9
49	All-Mechanical Polarization Control and Anomalous (Electro)Mechanical Responses in Ferroelectric Nanowires. Nano Letters, 2018, 18, 5996-6001.	9.1	9
50	Negative Linear Compressibility in Organicâ€"Inorganic Hybrid Perovskite [NH₂NH₃]X(HCOO)₃ (X = Mn, Fe, Co). Journal of Physical Chemistry Letters, 2022, 13, 3143-3149.	4.6	9
51	Negative Linear Compressibility in [NH₃NH₂]Co(HCOO)₃ and Its Structural Origin Revealed from First Principles. Journal of Physical Chemistry Letters, 2021, 12, 7560-7565.	4.6	8
52	Enhancement of electrocaloric response through quantum effects. Physical Review B, 2017, 96, .	3.2	7
53	Tuning the electrocaloric effect by varying Sr concentration in ferroelectric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="bold">Ba</mml:mi><mml:mrow><mml:mn mathvariant="bold-italic">1</mml:mn><mml:mo>âˆ'</mml:mo><mml:mi mathvariant="bold-italic">x</mml:mi></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="bold">Sr</mml:mi><mml:mi mathvariant="bold-italic">x</mml:mi></mml:msub><mml:msu	2.4	7
54	Relation between dielectric responses and polarization fluctuations in ferroelectric nanostructures. Physical Review B, 2007, 76, .	3.2	6

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55	Intrinsic dynamics of the electric-field-induced phase switching in antiferroelectric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>PbZrO</mml:mi><mml:mn>3</mml:mn></mml:msub></m ultrathin films. Physical Review B, 2018, 98, .	3.2	6
56	Comparative study of Minnesota functionals performance on ferroelectric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></m and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>PbTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review Materials, 2020, 4, .	2.4	6
57	Unusual Properties of Hydrogen-Bonded Ferroelectrics: The Case of Cobalt Formate. Physical Review Letters, 2022, 128, 077601.	7.8	6
58	Oscillatory Band Gap Behavior in Small Diameter Si-Clathrate Nanowires. Nano Letters, 2007, 7, 3424-3428.	9.1	5
59	Depolarizing field in temperature-graded ferroelectrics from an atomistic viewpoint. New Journal of Physics, 2013, 15, 043022.	2.9	5
60	Structural, Electrical, and Electromechanical Properties of Inverse Hybrid Perovskites from First-Principles: The Case of (CH₃NH₃)₃OI. Journal of Physical Chemistry C, 2021, 125, 8794-8802.	3.1	5
61	Chemically and electrically tunable spin polarization in ferroelectric Cd-based hybrid organic-inorganic perovskites. Physical Review B, 2021, 104, .	3.2	5
62	Unusual soft mode dynamics in ferroelectric PbTiO3 nanowire under different mechanical boundary conditions. Journal of Applied Physics, 2017, 122, .	2.5	4
63	Role of depolarization in the polarization reversal in ferroelectrics. Physical Review B, 2019, 100, .	3.2	4
64	Negative capacitance regime in ferroelectrics demystified from nonequilibrium molecular dynamics. Physical Review B, 2020, 102, .	3.2	4
65	The role of mechanical boundary conditions in the soft mode dynamics of PbTiO₃. Journal of Physics Condensed Matter, 2014, 26, 435901.	1.8	3
66	Nanoscale properties of PbZrO3 nanowires: Phase competition for enhanced energy conversion and storage. Computational Materials Science, 2016, 117, 468-471.	3.0	3
67	An unusual route to polarization reversal in ferroelectric ultrathin nanowires. Applied Physics Letters, 2014, 105, 012907.	3.3	2
68	Isentropic magnetoelectric coupling in planar heterostructures. Applied Physics Letters, 2017, 111, .	3.3	2