Inna Ponomareva

List of Publications by Year
in descending order

68	2,439	257450 24	197818 49
papers	citations	h-index	g-index

68	68	68	2120
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Unusual Properties of Hydrogen-Bonded Ferroelectrics: The Case of Cobalt Formate. Physical Review Letters, 2022, 128, 077601.	7.8	6
2	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
3	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
4	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
5	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
6	Chemically and electrically tunable spin polarization in ferroelectric Cd-based hybrid organic-inorganic perovskites. Physical Review B, 2021, 104, .	3.2	5
7	Negative capacitance regime in ferroelectrics demystified from nonequilibrium molecular dynamics. Physical Review B, 2020, 102, .	3.2	4
8	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
9	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
10	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
11	Role of depolarization in the polarization reversal in ferroelectrics. Physical Review B, 2019, 100, .	3.2	4
12	Unveiling Electrocaloric Potential of Antiferroelectrics with Phase Competition. Advanced Theory and Simulations, 2018, 1, 1800096.	2.8	9
13	High-frequency intrinsic dynamics of the electrocaloric effect from direct atomistic simulations. Physical Review B, 2018, 97, .	3.2	9
14	All-Mechanical Polarization Control and Anomalous (Electro)Mechanical Responses in Ferroelectric Nanowires. Nano Letters, 2018, 18, 5996-6001.	9.1	9
15	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 Physical Review B, 2018, 98, .	3.2	6
16	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>â^’</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
17	Electrocaloric effect in PbZrO3 thin films with antiferroelectric-ferroelectric phase competition. Computational Materials Science, 2017, 129, 44-48.	3.0	20
18	Unusual soft mode dynamics in ferroelectric PbTiO3 nanowire under different mechanical boundary conditions. Journal of Applied Physics, 2017, 122, .	2.5	4

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19	Isentropic magnetoelectric coupling in planar heterostructures. Applied Physics Letters, 2017, 111, .	3.3	2
20	Enhancement of electrocaloric response through quantum effects. Physical Review B, 2017, 96, .	3.2	7
21	Dynamics of antiferroelectric phase transition in PbZrO3. Physical Review B, 2017, 96, .	3.2	20
22	Emergence of ferroelectricity in antiferroelectric nanostructures. Nanotechnology, 2016, 27, 195705.	2.6	10
23	Nanoscale properties of PbZrO3 nanowires: Phase competition for enhanced energy conversion and storage. Computational Materials Science, 2016, 117, 468-471.	3.0	3
24	Elastocaloric Effect in Carbon Nanotubes and Graphene. Nano Letters, 2016, 16, 7008-7012.	9.1	24
25	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
26	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
27	Scaling law for electrocaloric temperature change in antiferroelectrics. Scientific Reports, 2016, 6, 19590.	3.3	20
28	Depolarizing field in ultrathin electrocalorics. Physical Review B, 2015, 92, .	3.2	9
29	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
30	Electrocaloric effect in ferroelectric nanowires from atomistic simulations. Scientific Reports, 2015, 5, 17294.	3.3	32
31	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> atomistic simulations. Physical Review B, 2015, 91, .	3.2	48
32	Thermally Mediated Mechanism to Enhance Magnetoelectric Coupling in Multiferroics. Physical Review Letters, 2015, 114, 177205.	7.8	20
33	Tailoring properties of ferroelectric ultrathin films by partial charge compensation. Applied Physics Letters, 2014, 104, .	3.3	22
34	An unusual route to polarization reversal in ferroelectric ultrathin nanowires. Applied Physics Letters, 2014, 105, 012907.	3.3	2
35	The role of mechanical boundary conditions in the soft mode dynamics of PbTiO₃. Journal of Physics Condensed Matter, 2014, 26, 435901.	1.8	3
36	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

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37	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
38	Terahertz sensing using ferroelectric nanowires. Nanotechnology, 2013, 24, 045501.	2.6	10
39	Depolarizing field in temperature-graded ferroelectrics from an atomistic viewpoint. New Journal of Physics, 2013, 15, 043022.	2.9	5
40	Emergence of central mode in the paraelectric phase of ferroelectric perovskites. MRS Communications, 2013, 3, 41-45.	1.8	20
41	Finite-temperature flexoelectricity in ferroelectric thin films from first principles. Physical Review B, 2012, 85, .	3.2	119
42	Bridging the Macroscopic and Atomistic Descriptions of the Electrocaloric Effect. Physical Review Letters, 2012, 108, 167604.	7.8	209
43	Competing polarization reversal mechanisms in ferroelectric nanowires. Physical Review B, 2012, 86, .	3.2	17
44	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:mml:	3.2	62
45	Nanodynamics of Ferroelectric Ultrathin Films. Physical Review Letters, 2011, 107, 177601.	7.8	27
46	Diffuse phase transitions in ferroelectric ultrathin films from first principles. Physical Review B, 2010, 81, .	3.2	11
47	Microscopic Insight into Temperature-Graded Ferroelectrics. Physical Review Letters, 2010, 105, 147602.	7.8	21
48	Low-Symmetry Phases in Ferroelectric Nanowires. Nano Letters, 2010, 10, 1177-1183.	9.1	62
49	Lattice dynamics in Ba_{0.7}Sr_{0.3}TiO₃: study by THz and IR spectroscopy andab initiosimulations. Phase Transitions, 2010, 83, 955-965.	1.3	10
50	Unusual static and dynamical characteristics of domain evolution in ferroelectric superlattices. Physical Review B, 2009, 79, .	3.2	34
51	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	3.2	79
52	Intrinsic electrocaloric effect in ferroelectric alloys from atomistic simulations. Physical Review B, 2009, 80, .	3.2	50
53	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
54	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

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55	Infrared and THz Soft-Mode Spectroscopy of (Ba,Sr)TiO3 Ceramics. Ferroelectrics, 2008, 367, 139-148.	0.6	13
56	Electrocaloric effect in bulk and low-dimensional ferroelectrics from first principles. Physical Review B, 2008, 78, .	3.2	76
57	Control of Vortices by Homogeneous Fields in Asymmetric Ferroelectric and Ferromagnetic Rings. Physical Review Letters, 2008, 100, 047201.	7.8	76
58	Nature of Dynamical Coupling between Polarization and Strain in Nanoscale Ferroelectrics from First Principles. Physical Review Letters, 2008, 101, 197602.	7.8	25
59	Relation between dielectric responses and polarization fluctuations in ferroelectric nanostructures. Physical Review B, 2007, 76, .	3.2	6
60	Thickness dependency of 180Â° stripe domains in ferroelectric ultrathin films: A first-principles-based study. Applied Physics Letters, 2007, 91, .	3.3	45
61	Dielectric Anomalies in Ferroelectric Nanostructures. Physical Review Letters, 2007, 99, 227601.	7.8	32
62	Thermal Conductivity in Thin Silicon Nanowires:Â Phonon Confinement Effect. Nano Letters, 2007, 7, 1155-1159.	9.1	170
63	Oscillatory Band Gap Behavior in Small Diameter Si-Clathrate Nanowires. Nano Letters, 2007, 7, 3424-3428.	9.1	5
64	Influence of the growth direction on properties of ferroelectric ultrathin films. Physical Review B, 2006, 74, .	3.2	29
65	Electric-Field-Induced Domain Evolution in Ferroelectric Ultrathin Films. Physical Review Letters, 2006, 96, 137602.	7.8	107
66	Low-dimensional ferroelectrics under different electrical and mechanical boundary conditions: Atomistic simulations. Physical Review B, 2005, 72, .	3.2	101
67	Atomistic treatment of depolarizing energy and field in ferroelectric nanostructures. Physical Review B, 2005, 72, .	3.2	132
68	Structure, Stability, and Quantum Conductivity of Small Diameter Silicon Nanowires. Physical Review Letters, 2005, 95, 265502.	7.8	67