Takahiro Shimada

List of Publications by Citations

167 papers	1,715 citations	23 h-index	32 g-index
177 ext. papers	1,994 ext. citations	4.1 avg, IF	4.98 L-index

#	Paper	IF	Citations
167	Hybrid Hartree-Fock density functional study of charged point defects in ferroelectric PbTiO3. *Physical Review B*, **2013**, 87,	3.3	55
166	Breakdown of continuum fracture mechanics at the nanoscale. *Scientific Reports*, **2015**, 5, 8596	4.9	53
165	Vacancy-driven ferromagnetism in ferroelectric PbTiO3. *Applied Physics Letters*, **2012**, 100, 162901	3.4	52
164	Stone-Wales transformations triggered by intrinsic localized modes in carbon nanotubes. *Physical Review B*, **2010**, 81,	3.3	52
163	Modulation of Gas Adsorption and Magnetic Properties of Monolayer-MoS2 by Antisite Defect and Strain. *Journal of Physical Chemistry C*, **2016**, 120, 14113-14121	3.8	51
162	Ab initio study of ferroelectric closure domains in ultrathin PbTiO3 films. *Physical Review B*, **2010**, 81,	3.3	48
161	Ab initio study of ferroelectricity in edged PbTiO3 nanowires under axial tension. *Physical Review B*, **2009**, 79,	3.3	47
160	Ab initio study of stress-induced domain switching in PbTiO3. *Physical Review B*, **2008**, 77,	3.3	41
159	Role of grain orientation distribution in the ferroelectric and ferroelastic domain switching of ferroelectric polycrystals. *Acta Materialia*, **2013**, 61, 6037-6049	8.4	38
158	Ab initio density functional theory study of strain effects on ferroelectricity at PbTiO3 surfaces. *Physical Review B*, **2006**, 74,	3.3	37
157	Multiferroic Domain Walls in Ferroelectric PbTiO3 with Oxygen Deficiency. *Nano Letters*, **2016**, 16, 454-8	11.5	36
156	Shell model potential for PbTiO3and its applicability to surfaces and domain walls. *Journal of Physics Condensed Matter*, **2008**, 20, 325225	1.8	35
155	Absence of ferroelectric critical size in ultrathin PbTiO3 nanotubes: a density-functional theory study. *Physical Review Letters*, **2012**, 108, 067601	7.4	34
154	Multiferroic nature of intrinsic point defects in BiFeO3: A hybrid Hartree-Fock density functional study. *Physical Review B*, **2016**, 93,	3.3	32
153	Large electrocaloric effect induced by the multi-domain to mono-domain transition in ferroelectrics. *Journal of Applied Physics*, **2014**, 115, 164102	2.5	32
152	Anomalous toughening in nanoscale ferroelectrics with polarization vortices. *Acta Materialia*, **2015**, 88, 147-155	8.4	31
151	Griffith Criterion for Nanoscale Stress Singularity in Brittle Silicon. *ACS Nano*, **2017**, 11, 6271-6276	16.7	30

150	Ferroelectricity in Ruddlesden-Popper Chalcogenide Perovskites for Photovoltaic Application: The Role of Tolerance Factor. *Journal of Physical Chemistry Letters*, **2017**, 8, 5834-5839	6.4	27
149	First-principles study of the interplay between grain boundaries and domain walls in ferroelectric PbTiO3. *Physical Review B*, **2011**, 83,	3.3	27
148	Switching the chirality of a ferroelectric vortex in designed nanostructures by a homogeneous electric field. *Physical Review B*, **2017**, 96,	3.3	26
147	Direct approach for flexoelectricity from first-principles calculations: cases for SrTiO3 and BaTiO3. *Journal of Physics Condensed Matter*, **2013**, 25, 415901	1.8	25
146	Hierarchical ferroelectric and ferrotoroidic polarizations coexistent in nano-metamaterials. *Scientific Reports*, **2015**, 5, 14653	4.9	25
145	Polar and toroidal electromechanical properties designed by ferroelectric nano-metamaterials. *Acta Materialia*, **2016**, 113, 81-89	8.4	24
144	Multiferroic grain boundaries in oxygen-deficient ferroelectric lead titanate. *Nano Letters*, **2015**, 15, 27-33	11.5	23
143	A unified and universal Griffith-based criterion for brittle fracture. *International Journal of Solids and Structures*, **2017**, 128, 67-72	3.1	23
142	Ab initio study of magnetism at iron surfaces under epitaxial in-plane strain. *Physical Review B*, **2010** , 81,	3.3	23
141	Mechanical control of magnetism in oxygen deficient perovskite SrTiO3. *Physical Chemistry Chemical Physics*, **2015**, 17, 27136-44	3.6	21
140	Multilevel hysteresis loop engineered with ferroelectric nano-metamaterials. *Acta Materialia*, **2017**, 125, 202-209	8.4	20
139	Emergence of ferromagnetism at a vacancy on a non-magnetic ferroelectric PbTiO3 surface: A first-principles study. *Acta Materialia*, **2012**, 60, 6322-6330	8.4	20
138	Coexistence of rectilinear and vortex polarizations at twist boundaries in ferroelectric PbTiO3 from first principles. *Physical Review B*, **2011**, 83,	3.3	20
137	Strain tunable ferroelectric and dielectric properties of BaZrO3. *Journal of Applied Physics*, **2014**, 115, 224107	2.5	19
136	Control of the polarity of magnetization vortex by torsion. *Applied Physics Letters*, **2013**, 103, 242413	3.4	19
135	Colossal magnetoelectric effect in 3-1 multiferroic nanocomposites originating from ultrafine nanodomain structures. *Applied Physics Letters*, **2015**, 107, 232904	3.4	19
134	An I-integral method for crack-tip intensity factor variation due to domain switching in ferroelectric single-crystals. *Journal of the Mechanics and Physics of Solids*, **2016**, 94, 207-229	5	19
133	Self-ordering of nontrivial topological polarization structures in nanoporous ferroelectrics. *Nanoscale*, **2017**, 9, 15525-15533	7.7	18

132	First-principles study on ferroelectricity at PbTiO3 surface steps. *Journal of Physics Condensed Matter*, **2010**, 22, 355901	1.8	18
131	Multiferroic Dislocations in Ferroelectric PbTiO. *Nano Letters*, **2017**, 17, 2674-2680	11.5	17
130	Ab initio study of multiferroic BiFeO3 (110) surfaces. *Physical Review B*, **2014**, 89,	3.3	16
129	Multiferroic Vacancies at Ferroelectric PbTiO(3) Surfaces. *Physical Review Letters*, **2015**, 115, 107202	7.4	16
128	Influence of nonlinear atomic interaction on excitation of intrinsic localized modes in carbon nanotubes. *Physica D: Nonlinear Phenomena*, **2010**, 239, 407-413	3.3	16
127	Instability criterion for ferroelectrics under mechanical/electric multi-fields: Ginzburg-Landau theory based modeling. *Acta Materialia*, **2016**, 112, 1-10	8.4	16
126	Disappearance of ferroelectric critical thickness in epitaxial ultrathin BaZrO3 films. *Physical Review B*, **2014**, 90,	3.3	15
125	Ab initio study of ferromagnetic single-wall nickel nanotubes. *Physical Review B*, **2011**, 84,	3.3	15
124	Ab initio study of spin-spiral noncollinear magnetism in a free-standing Fe(110) monolayer under in-plane strain. *Physical Review B*, **2012**, 85,	3.3	15
123	Strain-induced ferroelectricity and lattice coupling in BaSnO and SrSnO. *Physical Chemistry Chemical Physics*, **2017**, 19, 26047-26055	3.6	14
122	Simplified evaluation of mechanical instability in large-scale atomic structures. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2009**, 513-514, 166-171	5.3	14
121	Deterministic Switching of Polarization Vortices in Compositionally Graded Ferroelectrics Using a Mechanical Field. *Physical Review Applied*, **2019**, 11,	4.3	13
120	Defect-strain engineering for multiferroic and magnetoelectric properties in epitaxial (110) ferroelectric lead titanate. *Physical Review B*, **2015**, 92,	3.3	13
119	Challenge toward nanometer scale fracture mechanics. *Engineering Fracture Mechanics*, **2018**, 187, 33-44	4.2	13
118	Development of Interatomic Potential for Pb(Zr, Ti)O3 Based on Shell model. *Journal of Solid Mechanics and Materials Engineering*, **2007**, 1, 1423-1431		13
117	Strain energy density approach for brittle fracture from nano to macroscale and breakdown of continuum theory. *Theoretical and Applied Fracture Mechanics*, **2019**, 103, 102300	3.7	12
116	Effect of strain on the evolution of magnetic multi-vortices in ferromagnetic nano-platelets. *Journal of Physics Condensed Matter*, **2013**, 25, 226002	1.8	12
115	Unusual winding of helices under tension. *Applied Physics Letters*, **2014**, 105, 043702	3.4	12

114	Dislocation nucleation in a thin Cu film from molecular dynamics simulations: Instability activation by thermal fluctuations. *Physical Review B*, **2010**, 82,	3.3	12
113	Effect of geometric configuration on the electrocaloric properties of nanoscale ferroelectric materials. *Journal of Applied Physics*, **2018**, 123, 124103	2.5	11
112	Ab initio study of ferromagnetism in edged iron nanowires under axial strain. *Physical Review B*, **2011**, 84,	3.3	11
111	Asymmetric flux-closure domains in compositionally graded nanoscale ferroelectrics and unusual switching of toroidal ordering by an irrotational electric field. *Acta Materialia*, **2019**, 179, 215-223	8.4	10
110	Polar Superhelices in Ferroelectric Chiral Nanosprings. *Scientific Reports*, **2016**, 6, 35199	4.9	10
109	Chiral selectivity of unusual helimagnetic transition in iron nanotubes: chirality makes quantum helimagnets. *Nano Letters*, **2013**, 13, 2792-7	11.5	10
108	Fracture Nanomechanics		10
107	Magnetic instability criterion for spin□attice systems. *Computational Materials Science*, **2015**, 97, 216-221	3.2	9
106	Ferroelectric critical size and vortex domain structures of PbTiO3 nanodots: A density functional theory study. *Journal of Applied Physics*, **2018**, 123, 114101	2.5	9
105	Chiral selectivity of improper ferroelectricity in single-wall PbTiO3 nanotubes. *Physical Review B*, **2014**, 89,	3.3	9
104	Fracture Nanomechanics		9
103	Electron engineering of metallic multiferroic polarons in epitaxial BaTiO3. *Npj Computational Materials*, **2019**, 5,	10.9	8
102	Criterion of mechanical instabilities for dislocation structures. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2012**, 534, 681-687	5.3	8
101	Strain-induced improper ferroelectricity in Ruddlesden-Popper perovskite halides. *Physical Review B*, **2017**, 96,	3.3	8
100	Local suppression of ferroelectricity at PbTiO3 surface steps: a density functional theory study. *Journal of Physics Condensed Matter*, **2012**, 24, 045903	1.8	8
99	Mechanics of Fibrous Biological Materials With Hierarchical Chirality. *Journal of Applied Mechanics, Transactions ASME*, **2016**, 83,	2.7	8
98	Atomic investigation of effects of coating and confinement layer on laser shock peening. *Optics and Laser Technology*, **2020**, 131, 106409	4.2	7
97	Unusual Multiferroic Phase Transitions in PbTiO Nanowires. *Nano Letters*, **2016**, 16, 6774-6779	11.5	7

96	Ultrasoft silicon nanomembranes: thickness-dependent effective elastic modulus. *Nanoscale*, **2019**, 11, 15184-15194	7.7	7
95	Lifetime prediction of thermoelectric devices under thermal cycling. *Journal of Power Sources*, **2019** , 437, 226861	8.9	7
94	Strain-mediated multilevel ferroelectric random access memory operating through a magnetic field. *RSC Advances*, **2014**, 4, 45382-45388	3.7	7
93	Self-shaping of bioinspired chiral composites. *Acta Mechanica Sinica/Lixue Xuebao*, **2014**, 30, 533-539	2	7
92	Ferroelectric control of magnetic skyrmions in multiferroic heterostructures. *Physical Review B*, **2020**, 102,	3.3	7
91	Unusual Metallic Multiferroic Transitions in Electron-Doped PbTiO3. *Advanced Electronic Materials*, **2017**, 3, 1700134	6.4	6
90	Hybrid improper ferroelectricity in SrZrO3/BaZrO3 superlattice. *Physical Chemistry Chemical Physics* , **2016**, 18, 24024-32	3.6	6
89	Electron-beam irradiation alters bond strength in zinc oxide single crystal. *Applied Physics Letters*, **2020**, 116, 111902	3.4	5
88	Giant magnetoelectric effect at the graphone/ferroelectric interface. *Scientific Reports*, **2018**, 8, 12448	4.9	5
87	Effects of chirality and surface stresses on the bending and buckling of chiral nanowires. *Journal Physics D: Applied Physics*, **2014**, 47, 015302	3	5
86	Ferroelectricity at a junction structure of a 180□domain wall and a (001) surface in PbTiO3: A density functional theory study. *Physica B: Condensed Matter*, **2013**, 410, 22-27	2.8	5
85	Strain-induced polarity switching of magnetic vortex in Fe1□Gax alloys with different compositions. *Journal of Applied Physics*, **2014**, 115, 203911	2.5	5
84	Strain-induced phase transitions in multiferroic BiFeO3 . *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2012**, 376, 3368-3371	2.3	5
83	Multiphysics in Nanostructures. *Nanostructure Science and Technology*, **2017**,	0.9	5
82	Selective excitation of two-wave structure depending on crystal orientation under shock compression. *Science China: Physics, Mechanics and Astronomy*, **2020**, 63, 1	3.6	5
81	Electrocaloric effect enhancement in compositionally graded ferroelectric thin films driven by a needle-to-vortex domain structure transition. *Journal Physics D: Applied Physics*, **2021**, 54, 255307	3	5
80	Multiferroic Phases and Transitions in Ferroelectric Lead Titanate Nanodots. *Scientific Reports*, **2017**, 7, 45373	4.9	4
79	Continuum thermodynamics of unusual domain evolution-induced toughening effect in nanocracked strontium titanate. *Engineering Fracture Mechanics*, **2018**, 190, 232-244	4.2	4

78	Effect of the oxygen vacancy on the ferroelectricity of 90° domain wall structure in PbTiO3: A density functional theory study. *Journal of Applied Physics*, **2019**, 126, 174107	2.5	4
77	Development of Multi-Physics Instability Criterion for Atomic Structures and Application to Domain Switching in Ferroelectrics under External Electric Field. *Zairyo/Journal of the Society of Materials Science, Japan*, **2012**, 61, 155-161	0.1	4
76	Enhancement of electromechanical properties in (0-3) lead-free ferroelectric nanocomposites with multiphase coexistence. *Composites Communications*, **2020**, 22, 100540	6.7	4
75	Critical dimensional limit of continuum fracture mechanics for dislocation emission. *Engineering Fracture Mechanics*, **2016**, 163, 108-116	4.2	3
74	Multiferroic Transitions and Misfit Phase Diagram in Oxygen-Deficient Epitaxial (111) PbTiO3. *Advanced Electronic Materials*, **2016**, 2, 1600113	6.4	3
73	Periodically-arrayed ferroelectric nanostructures induced by dislocation structures in strontium titanate. *Physical Chemistry Chemical Physics*, **2019**, 21, 22756-22762	3.6	3
72	Unusual domain evolution in semiconducting ferroelectrics: A phase field study. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2013**, 377, 1643-1648	2.3	3
71	Ab initio study of shear strain effects on ferroelectricity at PbTiO3 thin films. *Surface Science*, **2012**, 606, 1331-1339	1.8	3
70	First-principles study of nanometer-sharp domain walls in ferromagnetic Fe monolayers under in-plane strain. *Journal of Physics Condensed Matter*, **2012**, 24, 095303	1.8	3
69	Development of Efficient Instability Analysis Method for Atomic Structures Using Linear Elements and Its Application to Amorphous Metal. *Journal of Solid Mechanics and Materials Engineering*, **2009**, 3, 807-818		3
68	Development of Efficient Instability Analysis Method for Atomic Structures Using Linear Elements and Its Application to Amorphous Metal. *Nihon Kikai Gakkai Ronbunshu, A Hen/Transactions of the Japan Society of Mechanical Engineers, Part A*, **2008**, 74, 1328-1335		3
67	Fracture Mechanics at Atomic Scales. *Advanced Structured Materials*, **2015**, 379-396	0.6	3
66	Investigation into the Breakdown of Continuum Fracture Mechanics at the Nanoscale: Synthesis of Recent Results on Silicon. *Structural Integrity*, **2019**, 205-210	0.2	3
65	Beyond conventional nonlinear fracture mechanics in graphene nanoribbons. *Nanoscale*, **2020**, 12, 18363-18370	7.7	3
64	An experimental study on atomic-level unified criterion for brittle fracture. *International Journal of Solids and Structures*, **2020**, 206, 1-8	3.1	3
63	Energy storage and dissipation of elastic-plastic deformation under shock compression: Simulation and Analysis. *Mechanics of Materials*, **2021**, 158, 103876	3.3	3
62	Phase field simulations on domain switching-induced toughening in ferromagnetic materials. *European Journal of Mechanics, A/Solids*, **2017**, 65, 205-211	3.7	2
61	Ferrotoroidic polarons in antiferrodistortive SrTiO3. *Physical Review B*, **2020**, 101,	3.3	2

60	Multi-physics analysis of nano-structured ferroelectrics by first-principles simulations. *Acta Mechanica*, **2013**, 224, 1261-1270	2.1	2
59	Hybrid functional study on the ferroelectricity of domain walls with O-vacancies in PbTiO3. *Mechanical Engineering Journal*, **2015**, 2, 15-00037-15-00037	0.5	2
58	Critical Thickness for Formation of Fatigue Dislocation Structures: A Discrete Dislocation Dynamics Study. *Nihon Kikai Gakkai Ronbunshu, A Hen/Transactions of the Japan Society of Mechanical Engineers, Part A*, **2012**, 78, 1242-1249		2
57	Development of Interatomic Potential for Pb(Zr,Ti)O3 Based on Shell Model. *Nihon Kikai Gakkai Ronbunshu, A Hen/Transactions of the Japan Society of Mechanical Engineers, Part A*, **2006**, 72, 817-822		2
56	In situ TEM observation of nanodomain mechanics in barium titanate under external loads. *Physical Review Materials*, **2020**, 4,	3.2	2
55	Defect engineering for nontrivial multiferroic orders in SrTiO3. *Physical Review Materials*, **2020**, 4,	3.2	2
54	Two-dimensional polar metal of a PbTe monolayer by electrostatic doping. *Nanoscale Horizons*, **2020**, 5, 1400-1406	10.8	2
53	Intrinsic and extrinsic effects on the electrotoroidic switching in a ferroelectric notched nanodot by a homogeneous electric field. *Physical Chemistry Chemical Physics*, **2019**, 21, 25011-25022	3.6	2
52	Prediction of tunable magnetoelectric properties in compositionally graded ferroelectric/ferromagnetic laminated nanocomposites. *Applied Physics Letters*, **2021**, 118, 052905	3.4	2
51	Linear-superelastic Ti-Nb nanocomposite alloys with ultralow modulus via high-throughput phase-field design and machine learning. *Npj Computational Materials*, **2021**, 7,	10.9	2
50	Interplay of coupling between strain and rotation in ferroelectric SrZrO3/SrTiO3 superlattices. *Journal of Physics Condensed Matter*, **2015**, 27, 385901	1.8	1
49	Multi-physics properties in ferroelectric nanostructure. *Mechanical Engineering Reviews*, **2014**, 1, SMM0009-SMM0009	1.7	1
48	First-Principles Study of Ferroelectric-Ferromagnetic Coupling in Multiferroic BiFeO3. *Zairyo/Journal of the Society of Materials Science, Japan*, **2014**, 63, 168-173	0.1	1
47	Instability Mode Analysis of Dislocation Nucleation from Notch Based on Atomistic Model : Instability Activation Mechanism under Finite Temperature. *Nihon Kikai Gakkai Ronbunshu, A Hen/Transactions of the Japan Society of Mechanical Engineers, Part A*, **2009**, 75, 1247-1254		1
46	Simplified Analysis of Mechanical Instability in Three-dimensional Atomic Components and Its Application to Nanoscale Crack. *Journal of Solid Mechanics and Materials Engineering*, **2010**, 4, 1071-1082		1
45	Mechanical Instability Criterion of Dislocation Structures Based on Discrete Dislocation Dynamics. *Nihon Kikai Gakkai Ronbunshu, A Hen/Transactions of the Japan Society of Mechanical Engineers, Part A*, **2010**, 76, 1721-1728		1
44	Abnormal Electromechanical Property of Nonlinearly Graded Lead-Free Ferroelectric Thin Films. *Advanced Theory and Simulations*, **2021**, 2100370	3.5	1
43	The rectilinear motion of the individual asymmetrical skyrmion driven by temperature gradients. *Acta Materialia*, **2021**, 221, 117383	8.4	1

42	Shock response and defect evolution of copper single crystals at room and elevated temperatures. *Modelling and Simulation in Materials Science and Engineering*, **2021**, 29, 045006	2	1
41	Topological ferroelectric nanostructures induced by mechanical strain in strontium titanate. *Physical Chemistry Chemical Physics*, **2019**, 21, 22420-22428	3.6	1
40	Interlaminar Fracture Toughness Measurement of Multilayered 2D Thermoelectric Materials Bi2Te3 by a Tapered Cantilever Bending Experiment. *Experimental Mechanics*, **2021**, 1	2.6	1
39	Reversible control of intrinsic shear strength of a ZnO single crystal through electron-beam-induced hole state. *Journal of Materials Research*, **2021**, 1	2.5	1
38	Flexoelectric properties of multilayer two-dimensional material MoS2. *Journal Physics D: Applied Physics*, **2022**, 55, 125302	3	1
37	Atomistic investigation on the conversion of plastic work to heat in high-rate shear deformation. *International Journal of Plasticity*, **2022**, 149, 103158	7.6	0
36	An Atomic-Level Unified Criterion for Brittle Fracture. *Structural Integrity*, **2020**, 334-336	0.2	
35	Periodically-arrayed ferroelectric nanostructures induced by strain concentration in SrTiO3. *Transactions of the JSME (in Japanese)*, **2019**, 85, 19-00175-19-00175	0.2	
34	First-principles Investigation of Edged Ferroelectric PbTiO3 Nanowires and the Role of Axial Strain. *Materials Research Society Symposia Proceedings*, **2009**, 1199, 147		
33	Fracture Nano-Mechanics : 1st Report, Interface Strength of Nano-Components(Thermal and Mechanical Reliability of Electronic Device and Mechanical Engineering). *Nihon Kikai Gakkai Ronbunshu, A Hen/Transactions of the Japan Society of Mechanical Engineers, Part A*, **2009**, 75, 778-783		
32	Fracture Nano-Mechanics : 2nd Report, Strength of Nano-Elements(Thermal and Mechanical Reliability of Electronic Device and Mechanical Engineering). *Nihon Kikai Gakkai Ronbunshu, A Hen/Transactions of the Japan Society of Mechanical Engineers, Part A*, **2009**, 75, 784-791		
31	632 Ab initio study of stress-induced domain switching in PbTiO_3. *The Proceedings of the Materials and Mechanics Conference*, **2007**, 2007, 489-490	0	
30	Thermomechanical conversion in high-rate plastic deformation of nanotwinned polycrystalline copper. *Journal of Thermal Stresses*, **2022**, 45, 65-80	2.2	
29	516 Development of Interatomic Potential for Pb(Zr,Ti)O_3 Based on Shell model. *The Proceedings of Conference of Kansai Branch*, **2005**, 2005.80, _5-37_-_5-38_	0	
28	272 Ab initio study of strain effects on ferroelectricity at PbTiO_3 surface. *The Proceedings of the Computational Mechanics Conference*, **2006**, 2006.19, 629-630	0	
27	811 Development of Interatomic Potential for PbTiO_3 Based on Shell model. *The Proceedings of the Computational Mechanics Conference*, **2007**, 2007.20, 263-264	0	
26	OS1203 First-principles Investigation on Domain Switching Mechanism in Lead Titanate. *The Proceedings of the Materials and Mechanics Conference*, **2008**, 2008, _OS1203-1_-_OS1203-2_	0	
25	236 Development of Efficient Instability Analysis Method for Atomic Structures Using Linear Elements and Its Application to Amorphous Metal. *The Proceedings of the Computational Mechanics Conference*, **2008**, 2008.21, 456-457	0	

24	OS0418 Ab initio study of ferroelectricity in edged PbTiO_3 nanowires under axial strain. *The Proceedings of the Materials and Mechanics Conference*, **2008**, 2008, _OS0418-1_-_OS0418-2_	0
23	210 Development of Shell Model Potential for PbTiO_3 and Applicability to Surfaces and Domain Walls. *The Proceedings of the Computational Mechanics Conference*, **2008**, 2008.21, 149-150	0
22	Ferroelectric critical size of SnTe nanoribbon and its mechanical strain engineering. *Transactions of the JSME (in Japanese)*, **2020**, 86, 19-00430-19-00430	0.2
21	One-dimensional atomic multiferroics by dislocation cores in nonmagnetic ferroelectric PbTiO3. *The Proceedings of the Materials and Mechanics Conference*, **2016**, 2016, OS11-16	0
20	Antiferroelectric and antiferrodistortive phase transitions in Ruddlesden-Popper Pb2TiO4from First-Principles. *Multiscale and Multiphysics Mechanics*, **2016**, 1, 233-244	
19	Ferroelectric Nanostructures. *Nanostructure Science and Technology*, **2017**, 97-139	0.9
18	Methodology of Quantum Mechanics/Atomic Simulations. *Nanostructure Science and Technology*, **2017**, 5-34	0.9
17	Multiferroic Nanostructures. *Nanostructure Science and Technology*, **2017**, 165-192	0.9
16	Strain Engineering on Nanosemiconductors. *Nanostructure Science and Technology*, **2017**, 67-96	0.9
15	Magnetism in Nanostructures. *Nanostructure Science and Technology*, **2017**, 141-164	0.9
14	Ideal Strength in Low-Dimensional Nanostructures. *Nanostructure Science and Technology*, **2017**, 35-66	0.9
13	Ferroic Nanometamaterials and Composites. *Nanostructure Science and Technology*, **2017**, 193-214	0.9
12	M2-2 Multi-physics Analysis on Ferroelectric PbTiO_3 Nanowires from First-principles (M2 MaterialCharacterization). *The Proceedings of the Symposium on Micro-Nano Science and Technology*, **2009**, 2009.1, 37-38	0
11	T0301-2-5 Development of Evaluation Method for Mechanical Instability Using Linear Elements and Its Application to Cracked Atomic Strcuture. *The Proceedings of the JSME Annual Meeting*, **2009**, 2009.8, 53-54	
10	1034 Ab initio study of multi-physics properties between magnetism and mechanical strain at Fe (001) thin films. *The Proceedings of the Computational Mechanics Conference*, **2009**, 2009.22, 300-301	0
9	1030 Ab initio study of ferroelectricity at PbTiO_3 surface step. *The Proceedings of the Computational Mechanics Conference*, **2009**, 2009.22, 292-293	0
8	1016 Ab initio study of ferroelectricity at twist boundary in PbTiO_3 and effect of strain. *The Proceedings of the Computational Mechanics Conference*, **2010**, 2010.23, 524-525	0
7	105 Ab initio study of magnetism in edged Fe nanowires under axial tension. *The Proceedings of Conference of Kansai Branch*, **2010**, 2010.85, _1-5_	0

6	1511 Molecular dynamics simulations on local defect nucleation triggered in carbon nanotubes by intrinsic localized modes. *The Proceedings of the Materials and Mechanics Conference*, **2010**, 2010, 99-101	0
5	OS1607 Development of magnetic instability criterion for atomic structures and its applications. *The Proceedings of the Materials and Mechanics Conference*, **2011**, 2011, _OS1607-1_-_OS1607-3_	0
4	318 A first-principles study of a nano-scale magnetic domain wall in an iron monolayer and the effect of in-plane strain. *The Proceedings of Conference of Kansai Branch*, **2012**, 2012.87, _3-29_	0
3	OS1206 Ab-initio Study of Emergence of Helimagnetism and Its Chiral Selectivity in Single-wall Iron Nanotubes. *The Proceedings of the Materials and Mechanics Conference*, **2013**, 2013, _OS1206-1_-_OS1206-3_	0
2	Deformation mode dependence of an exothermic chemical reaction in Ti/Si multilayered nanofilms. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing* , **2020**, 796, 140021	5.3
1	A unified atomic energy release rate criterion for nonlinear brittle fracture in graphene nanoribbons. *International Journal of Solids and Structures*, **2022**, 234-235, 111260	3.1