ElÄºf ErtekÄºn

List of Publications by Year
in descending order

99 papers	4,088 citations	186209 28 h-index	118793 62 g-index
107 all docs	107 docs citations	107 times ranked	5845 citing authors

#	Article	IF	Citations
1	Strain engineering and one-dimensional organization of metalâ€“insulator domains in single-crystal vanadium dioxide beams. Nature Nanotechnology, 2009, 4, 732-737.	15.6	562
2	New kagome prototype materials: discovery of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>KV</mml:mi><mml:mn>3</mml:mn></mml:, and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>CsV</mml:mi><mml:mn>3</mml:mn></m. Physical Review Materials, 2019, 3, .	0.9	398
3	Equilibrium limits of coherency in strained nanowire heterostructures. Journal of Applied Physics, 2005, 97, 114325.	1.1	337
4	Elastocaloric cooling capacity of shape memory alloys â€“ Role of deformation temperatures, mechanical cycling, stress hysteresis and inhomogeneity of transformation. Acta Materialia, 2017, 135, 158-176.	3.8	172
5	Elastocaloric cooling potential of NiTi, Ni2FeGa, and CoNiAl. Acta Materialia, 2015, 96, 420-427.	3.8	169
6	Ultrasoft slip-mediated bending in few-layer graphene. Nature Materials, 2020, 19, 305-309.	13.3	159
7	Phonon transport on two-dimensional graphene/boron nitride superlattices. Physical Review B, 2014, 90, .	1.1	157
8	Photocatalytic Reaction Centers in Two-Dimensional Titanium Oxide Crystals. Journal of the American Chemical Society, 2015, 137, 239-244.	6.6	148
9	Insulator-to-Metal Transition in Selenium-Hyperdoped Silicon: Observation and Origin. Physical Review Letters, 2012, 108, 026401.	2.9	141
10	Phonons, Localization, and Thermal Conductivity of Diamond Nanothreads and Amorphous Graphene. Nano Letters, 2016, 16, 4763-4772.	4.5	129
11	Resolving anomalous strain effects on two-dimensional phonon flows: The cases of graphene, boron nitride, and planar superlattices. Physical Review B, 2015, 91, .	1.1	84
12	Topological description of the Stone-Wales defect formation energy in carbon nanotubes and graphene. Physical Review B, 2009, 79, .	1.1	83
13	A Cocatalyst that Stabilizes a Hydride Intermediate during Photocatalytic Hydrogen Evolution over a Rhodiumâ€Doped TiO₂ Nanosheet. Angewandte Chemie - International Edition, 2018, 57, 9073-9077.	7.2	62
14	Generalized Debye-Peierls/Allen-Feldman model for the lattice thermal conductivity of low-dimensional and disordered materials. Physical Review B, 2016, 93, .	1.1	58
15	Atomically precise graphene etch stops for three dimensional integrated systems from two dimensional material heterostructures. Nature Communications, 2018, 9, 3988.	5.8	56
16	Elastocaloric effects in the extreme. Scripta Materialia, 2018, 148, 122-126.	2.6	54
17	Point-defect optical transitions and thermal ionization energies from quantum Monte Carlo methods: Application to the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>F</mml:mi></mml:math>-center defect in MgO. Physical Review B, 2013, 87, .	1.1	53
18	Mixed phononic and non-phononic transport in hybrid lead halide perovskites: glass-crystal duality, dynamical disorder, and anharmonicity. Energy and Environmental Science, 2019, 12, 216-229.	15.6	51

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19	Ripples, Strain, and Misfit Dislocations: Structure of Grapheneâ€“Boron Nitride Superlattice Interfaces. Nano Letters, 2015, 15, 1468-1475.	4.5	49
20	Interplay between intrinsic defects, doping, and free carrier concentration in SrTiO<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>thin films. Physical Review B, 2012, 85, .	1.1	46
21	Asynchronous Photoexcited Electronic and Structural Relaxation in Lead-Free Perovskites. Journal of the American Chemical Society, 2019, 141, 13074-13080.	6.6	39
22	Achieving a Carbon Neutral Future through Advanced Functional Materials and Technologies. Bulletin of the Chemical Society of Japan, 2022, 95, 73-103.	2.0	39
23	Towards a systematic assessment of errors in diffusion Monte Carlo calculations of semiconductors: Case study of zinc selenide and zinc oxide. Journal of Chemical Physics, 2015, 143, 224707.	1.2	36
24	Superelastic metal-insulator phase transition in single-crystal<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>VO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu Physical Review B, 2009, 80, .	1.1	34
25	Phase stability and properties of manganese oxide polymorphs: Assessment and insights from diffusion Monte Carlo. Physical Review B, 2015, 92, .	1.1	33
26	Plastic deformation of B2-NiTi â€“ is it slip or twinning?. Philosophical Magazine Letters, 2017, 97, 217-228.	0.5	32
27	Designing the Bending Stiffness of 2D Material Heterostructures. Advanced Materials, 2021, 33, e2007269.	11.1	31
28	Designing Optimal Perovskite Structure for High Ionic Conduction. Advanced Materials, 2020, 32, e1905178.	11.1	30
29	Mechanism and energetics of O and O2 adsorption on polar and non-polar ZnO surfaces. Journal of Chemical Physics, 2016, 144, 184708.	1.2	28
30	Ultralow Thermal Conductivity in Diamond-Like Semiconductors: Selective Scattering of Phonons from Antisite Defects. Chemistry of Materials, 2018, 30, 3395-3409.	3.2	28
31	Ideal torsional strengths and stiffnesses of carbon nanotubes. Physical Review B, 2005, 72, .	1.1	27
32	Carrier density control in Cu2HgGeTe4and discovery of Hg2GeTe4viaphase boundary mapping. Journal of Materials Chemistry A, 2019, 7, 621-631.	5.2	27
33	Toward design of cation transport in solid-state battery electrolytes: Structure-dynamics relationships. Current Opinion in Solid State and Materials Science, 2020, 24, 100875.	5.6	27
34	Facets of nanotube synthesis: High-resolution transmission electron microscopy study and density functional theory calculations. Physical Review B, 2009, 79, .	1.1	26
35	Extended X-ray absorption fine structure spectroscopy of selenium-hyperdoped silicon. Journal of Applied Physics, 2013, 114, 133507.	1.1	25
36	Surface-assisted defect engineering of point defects in ZnO. Applied Physics Letters, 2016, 108, 241603.	1.5	24

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37	Fixed-node diffusion Monte Carlo description of nitrogen defects in zinc oxide. Physical Review B, 2017, 95, .	1.1	21
38	Vibrational Energy Transport in Hybrid Ordered/Disordered Nanocomposites: Hybridization and Avoided Crossings of Localized and Delocalized Modes. Advanced Functional Materials, 2018, 28, 1706268.	7.8	21
39	New n-Type Zintl Phases for Thermoelectrics: Discovery, Structural Characterization, and Band Engineering of the Compounds A₂CdP₂ (A = Sr, Ba, Eu). Chemistry of Materials, 2020, 32, 10697-10707.	3.2	21
40	Thermoelectric phonon-glass electron-crystal via ion beam patterning of silicon. Physical Review B, 2018, 97, .	1.1	20
41	Computational Analysis of the Interplay between Deep Level Traps and Perovskite Solar Cell Efficiency. Journal of the American Chemical Society, 2018, 140, 15655-15660.	6.6	20
42	Atomistic Mechanisms for the Thermal Relaxation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Au</mml:mi></mml:math> -hyperdoped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Si</mml:mi></mml:math>. Physical Review Applied, 2019, 12, .	1.5	20
43	Identifying Charge Transfer Mechanisms across Semiconductor Heterostructures via Surface Dipole Modulation and Multiscale Modeling. Journal of the American Chemical Society, 2018, 140, 13223-13232.	6.6	19
44	Plasticity in carbon nanotubes: Cooperative conservative dislocation motion. Physical Review B, 2010, 81, .	1.1	18
45	Atomic scale origins of sub-band gap optical absorption in gold-hyperdoped silicon. AIP Advances, 2018, 8, 055014.	0.6	18
46	Evidence for vacancy trapping in Au-hyperdoped Si following pulsed laser melting. APL Materials, 2019, 7, .	2.2	18
47	Material-Dependent Evolution of Mechanical Folding Instabilities in Two-Dimensional Atomic Membranes. ACS Applied Materials & Interfaces, 2020, 12, 10801-10808.	4.0	18
48	Native Defect Engineering in CuInTe₂. Chemistry of Materials, 2021, 33, 359-369.	3.2	18
49	Origins and Control of Optical Absorption in a Nondilute Oxide Solid Solution: Sr(Ti,Fe)O_{3â€“x} Perovskite Case Study. Chemistry of Materials, 2019, 31, 1030-1041.	3.2	17
50	Correlating Surface Crystal Orientation and Gas Kinetics in Perovskite Oxide Electrodes. Advanced Materials, 2021, 33, e2100977.	11.1	17
51	Interplay of Wetting and Elasticity in the Nucleation of Carbon Nanotubes. Physical Review Letters, 2011, 107, 185503.	2.9	16
52	Stochastic Stress Jumps Due to Soliton Dynamics in Two-Dimensional van der Waals Interfaces. Nano Letters, 2020, 20, 1201-1207.	4.5	16
53	Structural and thermal effects of ion-irradiation induced defect configurations in silicon. Physical Review B, 2017, 95, .	1.1	15
54	Two-Dimensional TiO₂ Nanosheets for Photo and Electro-Chemical Oxidation of Water: Predictions of Optimal Dopant Species from First-Principles. Journal of Physical Chemistry C, 2017, 121, 19201-19208.	1.5	14

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55	Multiscale Computational Design of Functionalized Photocathodes for H₂ Generation. Journal of the American Chemical Society, 2018, 140, 50-53.	6.6	14
56	A Cocatalyst that Stabilizes a Hydride Intermediate during Photocatalytic Hydrogen Evolution over a Rhodiumâ€Doped TiO₂ Nanosheet. Angewandte Chemie, 2018, 130, 9211-9215.	1.6	14
57	Doping by design: finding new n-type dopable ABX₄ Zintl phases for thermoelectrics. Journal of Materials Chemistry A, 2020, 8, 25306-25315.	5.2	14
58	Effect of Surface Coverage and Composition on the Stability and Interfacial Dipole of Functionalized Silicon. Journal of Physical Chemistry C, 2017, 121, 11312-11318.	1.5	13
59	Atomic Modeling and Electronic Structure of Mixed Ionicâ€“Electronic Conductor SrTi1â€“xFexO3â€“x/2+Î´ Considered as a Mixture of SrTiO3 and Sr2Fe2O5. Chemistry of Materials, 2019, 31, 233-243.	3.2	13
60	Tuning p-Si(111) Photovoltage via Molecule|Semiconductor Electronic Coupling. Journal of the American Chemical Society, 2021, 143, 2567-2580.	6.6	13
61	Lattice mismatch induced ripples and wrinkles in planar graphene/boron nitride superlattices. Journal of Applied Physics, 2015, 117, .	1.1	12
62	Computational insights into charge transfer across functionalized semiconductor surfaces. Science and Technology of Advanced Materials, 2017, 18, 681-692.	2.8	12
63	First-principles description of oxygen self-diffusion in rutile TiO₂: assessment of uncertainties due to enthalpy and entropy contributions. Physical Chemistry Chemical Physics, 2018, 20, 17448-17457.	1.3	12
64	Topologically derived dislocation theory for twist and stretch moirÃ© superlattices in bilayer graphene. Physical Review B, 2020, 102, .	1.1	12
65	Screened-exchange density functional theory description of the electronic structure and phase stability of the chalcopyrite materials<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>AgInSe</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>AuInSe</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2016, 93, .	1.1	11
66	Asymmetric response of ferroelectric/metal oxide heterojunctions for catalysis arising from interfacial chemistry. Physical Chemistry Chemical Physics, 2017, 19, 5870-5879.	1.3	11
67	Symmetry breaking in Ge_{1â€“x}Mn_xTe and the impact on thermoelectric transport. Journal of Materials Chemistry A, 2022, 10, 16468-16477.	5.2	11
68	Grain boundary structure and migration in graphene via the displacement shift complete lattice. Acta Materialia, 2019, 166, 67-74.	3.8	10
69	A Novel, Layered Phase in Tiâ€Rich SrTiO₃ Epitaxial Thin Films. Advanced Materials, 2015, 27, 861-868.	11.1	9
70	Accurate tight-binding model for twisted bilayer graphene describes topological flat bands without geometric relaxation. Physical Review B, 2022, 105, .	1.1	9
71	Equilibrium Analysis of Lattice-Mismatched Nanowire Heterostructures. Materials Research Society Symposia Proceedings, 2002, 737, 262.	0.1	8
72	Elasticity theory of topological defects in carbon nanotubes and graphene. Philosophical Magazine Letters, 2008, 88, 159-167.	0.5	8

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73	Computational Approaches to Photoelectrode Design through Molecular Functionalization for Enhanced Photoelectrochemical Water Splitting. ChemSusChem, 2019, 12, 1858-1871.	3.6	8
74	Perovskite Na-ion conductors developed from analogous Li3xLa2/3â˜xTiO3 (LLTO): chemo-mechanical and defect engineering. Journal of Materials Chemistry A, 2021, 9, 21241-21258.	5.2	7
75	Effect of substrate and lid on the optical response of an axially excited slab of a dielectric thin-film helicoidal bianisotropic medium. Microwave and Optical Technology Letters, 1999, 20, 218-222.	0.9	6
76	Optical interconnects realizable with thinâ€“film helicoidal bianisotropic mediums. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2001, 457, 817-836.	1.0	6
77	Cluster Expansion Framework for the Sr(Ti1â€“xFex)O3â€“x/2 (0 < x < 1) Mixed Ionic Electronic Conductor: Properties Based on Realistic Configurations. Chemistry of Materials, 2019, 31, 3144-3153.	3.2	6
78	Kinetic Control of Oxygen Interstitial Interaction with TiO₂(110) via the Surface Fermi Energy. Langmuir, 2020, 36, 12632-12648.	1.6	6
79	Tuning valley degeneracy with band inversion. Journal of Materials Chemistry A, 2022, 10, 1588-1595.	5.2	6
80	Reducing extrinsic damping of surface acoustic waves at gigahertz frequencies. Journal of Applied Physics, 2016, 119, .	1.1	5
81	Fermi level dependence of gasâ€“solid oxygen defect exchange mechanism on TiO2 (110) by first-principles calculations. Journal of Chemical Physics, 2020, 153, 124710.	1.2	5
82	Crowd-Sourced Data and Analysis Tools for Advancing the Chemical Vapor Deposition of Graphene: Implications for Manufacturing. ACS Applied Nano Materials, 2020, 3, 10144-10155.	2.4	5
83	First-Principle Study of the Electronic Structure and Stability of Reconstructed AgInSe2 (112) Polar Surfaces. IEEE Journal of Photovoltaics, 2017, 7, 1781-1788.	1.5	4
84	Mechanism of creation and destruction of oxygen interstitial atoms by nonpolar zinc oxide(101Ì„0) surfaces. Physical Chemistry Chemical Physics, 2021, 23, 16423-16435.	1.3	4
85	Pathways to controlled 3D deformation of graphene: Manipulating the motion of topological defects. Current Opinion in Solid State and Materials Science, 2021, 25, 100893.	5.6	4
86	Controlling thermoelectric transport via native defects in the diamond-like semiconductors Cu2HgGeTe4 and Hg2GeTe4. Journal of Materials Chemistry A, 0, , .	5.2	4
87	Carrier Dynamics and Absorption Properties of Gold-Hyperdoped Germanium: Insight Into Tailoring Defect Energetics. Physical Review Applied, 2021, 15, .	1.5	3
88	Understanding Cu incorporation in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Cu</mml:mi><mml:mrow><mml:mn>2</mml:mn> structure using resonant x-ray diffraction. Physical Review Materials, 2021, 5, .	0.9	3
89	Toward Zero-Strain Mixed Conductors: Anomalously Low Redox Coefficients of Chemical Expansion in Praseodymium-Oxide Perovskites. Chemistry of Materials, 0, , .	3.2	3
90	Surface-Based Post-synthesis Manipulation of Point Defects in Metal Oxides Using Liquid Water. ACS Applied Materials & Interfaces, 2022, 14, 34059-34068.	4.0	3

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91	Light on the path. Nature Catalysis, 2018, 1, 240-241.	16.1	2
92	Design Strategy for the Molecular Functionalization of Semiconductor Photoelectrodes: A Case Study of p-Si(111) Photocathodes for H₂ Generation. Langmuir, 2018, 34, 2959-2966.	1.6	2
93	Anomalous electronic properties in layered, disordered ZnVSb. Physical Review Materials, 2021, 5, .	0.9	2
94	Structural defects in compounds <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Zn</mml:mi><mml:mi>X</mml:mi><mml:mi>Sb</mml:mi><mml:mi><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mo>(</mml:mo><mml:mi>X</mml:mi><mml:mo>=</mml:mo><mml:mi>C : Origin of disorder and its relationship with electronic pro. Physical Review Materials, 2022, 6, .	0.9	2
95	Infrared thermography videos of the elastocaloric effect for shape memory alloys NiTi and Ni 2 FeGa. Data in Brief, 2015, 5, 7-8.	0.5	1
96	Probing The Mechanical Properties of Few-Layer Graphene with Aberration-Corrected, Low-Voltage STEM. Microscopy and Microanalysis, 2019, 25, 1730-1731.	0.2	0
97	2D Materials: Designing the Bending Stiffness of 2D Material Heterostructures (Adv. Mater. 9/2021). Advanced Materials, 2021, 33, 2170066.	11.1	0
98	Multisublattice cluster expansion study of short-range ordering in iron-substituted strontium titanate. Computational Materials Science, 2022, 202, 110969.	1.4	0
99	Carrier Lifetime of Au-Hyperdoped Ge using Terahertz Spectroscopy. , 2020, , .		0