ElÄºf ErtekÄºn

List of Publications by Year
in descending order

99 papers	4,088 citations	186265 28 h-index	118850 62 g-index
107 all docs	107 docs citations	107 times ranked	5845 citing authors

#	Article	IF	Citations
1	Multisublattice cluster expansion study of short-range ordering in iron-substituted strontium titanate. Computational Materials Science, 2022, 202, 110969.	3.0	0
2	Tuning valley degeneracy with band inversion. Journal of Materials Chemistry A, 2022, 10, 1588-1595.	10.3	6
3	Achieving a Carbon Neutral Future through Advanced Functional Materials and Technologies. Bulletin of the Chemical Society of Japan, 2022, 95, 73-103.	3.2	39
4	Accurate tight-binding model for twisted bilayer graphene describes topological flat bands without geometric relaxation. Physical Review B, 2022, 105, .	3.2	9
5	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: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, .	2.4	2
6	Symmetry breaking in Ge_{1â^'x}Mn_xTe and the impact on thermoelectric transport. Journal of Materials Chemistry A, 2022, 10, 16468-16477.	10.3	11
7	Surface-Based Post-synthesis Manipulation of Point Defects in Metal Oxides Using Liquid Water. ACS Applied Materials & Interfaces, 2022, 14, 34059-34068.	8.0	3
8	Native Defect Engineering in CuInTe₂. Chemistry of Materials, 2021, 33, 359-369.	6.7	18
9	Designing the Bending Stiffness of 2D Material Heterostructures. Advanced Materials, 2021, 33, e2007269.	21.0	31
10	Anomalous electronic properties in layered, disordered ZnVSb. Physical Review Materials, 2021, 5, .	2.4	2
11	Mechanism of creation and destruction of oxygen interstitial atoms by nonpolar zinc oxide(101Ì„0) surfaces. Physical Chemistry Chemical Physics, 2021, 23, 16423-16435.	2.8	4
12	Tuning p-Si(111) Photovoltage via Molecule|Semiconductor Electronic Coupling. Journal of the American Chemical Society, 2021, 143, 2567-2580.	13.7	13
13	2D Materials: Designing the Bending Stiffness of 2D Material Heterostructures (Adv. Mater. 9/2021). Advanced Materials, 2021, 33, 2170066.	21.0	0
14	Pathways to controlled 3D deformation of graphene: Manipulating the motion of topological defects. Current Opinion in Solid State and Materials Science, 2021, 25, 100893.	11.5	4
15	Correlating Surface Crystal Orientation and Gas Kinetics in Perovskite Oxide Electrodes. Advanced Materials, 2021, 33, e2100977.	21.0	17
16	Carrier Dynamics and Absorption Properties of Gold-Hyperdoped Germanium: Insight Into Tailoring Defect Energetics. Physical Review Applied, 2021, 15, .	3.8	3
17	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, .	2.4	3
18	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.	10.3	7

#	Article	IF	Citations
19	Ultrasoft slip-mediated bending in few-layer graphene. Nature Materials, 2020, 19, 305-309.	27.5	159
20	Designing Optimal Perovskite Structure for High Ionic Conduction. Advanced Materials, 2020, 32, e1905178.	21.0	30
21	Kinetic Control of Oxygen Interstitial Interaction with TiO₂(110) via the Surface Fermi Energy. Langmuir, 2020, 36, 12632-12648.	3.5	6
22	Toward design of cation transport in solid-state battery electrolytes: Structure-dynamics relationships. Current Opinion in Solid State and Materials Science, 2020, 24, 100875.	11.5	27
23	Fermi level dependence of gasâ€“solid oxygen defect exchange mechanism on TiO2 (110) by first-principles calculations. Journal of Chemical Physics, 2020, 153, 124710.	3.0	5
24	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.	5.0	5
25	Doping by design: finding new n-type dopable ABX₄ Zintl phases for thermoelectrics. Journal of Materials Chemistry A, 2020, 8, 25306-25315.	10.3	14
26	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.	6.7	21
27	Topologically derived dislocation theory for twist and stretch moirÃ© superlattices in bilayer graphene. Physical Review B, 2020, 102, .	3.2	12
28	Material-Dependent Evolution of Mechanical Folding Instabilities in Two-Dimensional Atomic Membranes. ACS Applied Materials & Interfaces, 2020, 12, 10801-10808.	8.0	18
29	Stochastic Stress Jumps Due to Soliton Dynamics in Two-Dimensional van der Waals Interfaces. Nano Letters, 2020, 20, 1201-1207.	9.1	16
30	Carrier Lifetime of Au-Hyperdoped Ge using Terahertz Spectroscopy. , 2020, , .		0
31	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, .	3.8	20
32	Asynchronous Photoexcited Electronic and Structural Relaxation in Lead-Free Perovskites. Journal of the American Chemical Society, 2019, 141, 13074-13080.	13.7	39
33	Probing The Mechanical Properties of Few-Layer Graphene with Aberration-Corrected, Low-Voltage STEM. Microscopy and Microanalysis, 2019, 25, 1730-1731.	0.4	0
34	Carrier density control in Cu2HgGeTe4and discovery of Hg2GeTe4viaphase boundary mapping. Journal of Materials Chemistry A, 2019, 7, 621-631.	10.3	27
35	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.	30.8	51
36	Computational Approaches to Photoelectrode Design through Molecular Functionalization for Enhanced Photoelectrochemical Water Splitting. ChemSusChem, 2019, 12, 1858-1871.	6.8	8

#	Article	IF	Citations
37	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.	6.7	6
38	Evidence for vacancy trapping in Au-hyperdoped Si following pulsed laser melting. APL Materials, 2019, 7, .	5.1	18
39	Grain boundary structure and migration in graphene via the displacement shift complete lattice. Acta Materialia, 2019, 166, 67-74.	7.9	10
40	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.	6.7	17
41	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.	6.7	13
42	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, .	2.4	398
43	Vibrational Energy Transport in Hybrid Ordered/Disordered Nanocomposites: Hybridization and Avoided Crossings of Localized and Delocalized Modes. Advanced Functional Materials, 2018, 28, 1706268.	14.9	21
44	Light on the path. Nature Catalysis, 2018, 1, 240-241.	34.4	2
45	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.	3.5	2
46	Multiscale Computational Design of Functionalized Photocathodes for H₂ Generation. Journal of the American Chemical Society, 2018, 140, 50-53.	13.7	14
47	Ultralow Thermal Conductivity in Diamond-Like Semiconductors: Selective Scattering of Phonons from Antisite Defects. Chemistry of Materials, 2018, 30, 3395-3409.	6.7	28
48	Thermoelectric phonon-glass electron-crystal via ion beam patterning of silicon. Physical Review B, 2018, 97, .	3.2	20
49	Elastocaloric effects in the extreme. Scripta Materialia, 2018, 148, 122-126.	5.2	54
50	Atomically precise graphene etch stops for three dimensional integrated systems from two dimensional material heterostructures. Nature Communications, 2018, 9, 3988.	12.8	56
51	Identifying Charge Transfer Mechanisms across Semiconductor Heterostructures via Surface Dipole Modulation and Multiscale Modeling. Journal of the American Chemical Society, 2018, 140, 13223-13232.	13.7	19
52	Computational Analysis of the Interplay between Deep Level Traps and Perovskite Solar Cell Efficiency. Journal of the American Chemical Society, 2018, 140, 15655-15660.	13.7	20
53	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.	13.8	62
54	Atomic scale origins of sub-band gap optical absorption in gold-hyperdoped silicon. AIP Advances, 2018, 8, 055014.	1.3	18

#	Article	IF	Citations
55	A Cocatalyst that Stabilizes a Hydride Intermediate during Photocatalytic Hydrogen Evolution over a Rhodiumâ€Doped TiO₂ Nanosheet. Angewandte Chemie, 2018, 130, 9211-9215.	2.0	14
56	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.	2.8	12
57	Asymmetric response of ferroelectric/metal oxide heterojunctions for catalysis arising from interfacial chemistry. Physical Chemistry Chemical Physics, 2017, 19, 5870-5879.	2.8	11
58	Fixed-node diffusion Monte Carlo description of nitrogen defects in zinc oxide. Physical Review B, 2017, 95, .	3.2	21
59	Plastic deformation of B2-NiTi â€“ is it slip or twinning?. Philosophical Magazine Letters, 2017, 97, 217-228.	1.2	32
60	Effect of Surface Coverage and Composition on the Stability and Interfacial Dipole of Functionalized Silicon. Journal of Physical Chemistry C, 2017, 121, 11312-11318.	3.1	13
61	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.	7.9	172
62	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.	3.1	14
63	Computational insights into charge transfer across functionalized semiconductor surfaces. Science and Technology of Advanced Materials, 2017, 18, 681-692.	6.1	12
64	Structural and thermal effects of ion-irradiation induced defect configurations in silicon. Physical Review B, 2017, 95, .	3.2	15
65	First-Principle Study of the Electronic Structure and Stability of Reconstructed AgInSe2 (112) Polar Surfaces. IEEE Journal of Photovoltaics, 2017, 7, 1781-1788.	2.5	4
66	Phonons, Localization, and Thermal Conductivity of Diamond Nanothreads and Amorphous Graphene. Nano Letters, 2016, 16, 4763-4772.	9.1	129
67	Surface-assisted defect engineering of point defects in ZnO. Applied Physics Letters, 2016, 108, 241603.	3.3	24
68	Reducing extrinsic damping of surface acoustic waves at gigahertz frequencies. Journal of Applied Physics, 2016, 119, .	2.5	5
69	Mechanism and energetics of O and O2 adsorption on polar and non-polar ZnO surfaces. Journal of Chemical Physics, 2016, 144, 184708.	3.0	28
70	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><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, .	3.2	11
71	Generalized Debye-Peierls/Allen-Feldman model for the lattice thermal conductivity of low-dimensional and disordered materials. Physical Review B, 2016, 93, .	3.2	58
72	Infrared thermography videos of the elastocaloric effect for shape memory alloys NiTi and Ni 2 FeGa. Data in Brief, 2015, 5, 7-8.	1.0	1

#	Article	IF	Citations
73	Phase stability and properties of manganese oxide polymorphs: Assessment and insights from diffusion Monte Carlo. Physical Review B, 2015, 92, .	3.2	33
74	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.	3.0	36
75	Lattice mismatch induced ripples and wrinkles in planar graphene/boron nitride superlattices. Journal of Applied Physics, 2015, 117, .	2.5	12
76	Ripples, Strain, and Misfit Dislocations: Structure of Grapheneâ€“Boron Nitride Superlattice Interfaces. Nano Letters, 2015, 15, 1468-1475.	9.1	49
77	Resolving anomalous strain effects on two-dimensional phonon flows: The cases of graphene, boron nitride, and planar superlattices. Physical Review B, 2015, 91, .	3.2	84
78	Elastocaloric cooling potential of NiTi, Ni2FeGa, and CoNiAl. Acta Materialia, 2015, 96, 420-427.	7.9	169
79	A Novel, Layered Phase in Tiâ€Rich SrTiO₃ Epitaxial Thin Films. Advanced Materials, 2015, 27, 861-868.	21.0	9
80	Photocatalytic Reaction Centers in Two-Dimensional Titanium Oxide Crystals. Journal of the American Chemical Society, 2015, 137, 239-244.	13.7	148
81	Phonon transport on two-dimensional graphene/boron nitride superlattices. Physical Review B, 2014, 90, .	3.2	157
82	Extended X-ray absorption fine structure spectroscopy of selenium-hyperdoped silicon. Journal of Applied Physics, 2013, 114, 133507.	2.5	25
83	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, .	3.2	53
84	Insulator-to-Metal Transition in Selenium-Hyperdoped Silicon: Observation and Origin. Physical Review Letters, 2012, 108, 026401.	7.8	141
85	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, .	3.2	46
86	Interplay of Wetting and Elasticity in the Nucleation of Carbon Nanotubes. Physical Review Letters, 2011, 107, 185503.	7.8	16
87	Plasticity in carbon nanotubes: Cooperative conservative dislocation motion. Physical Review B, 2010, 81, .	3.2	18
88	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, .	3.2	34
89	Facets of nanotube synthesis: High-resolution transmission electron microscopy study and density functional theory calculations. Physical Review B, 2009, 79, .	3.2	26
90	Strain engineering and one-dimensional organization of metalâ€“insulator domains in single-crystal vanadium dioxide beams. Nature Nanotechnology, 2009, 4, 732-737.	31.5	562

#	ARTICLE	IF	CITATIONS
91	Topological description of the Stone-Wales defect formation energy in carbon nanotubes and graphene. Physical Review B, 2009, 79, .	3.2	83
92	Elasticity theory of topological defects in carbon nanotubes and graphene. Philosophical Magazine Letters, 2008, 88, 159-167.	1.2	8
93	Ideal torsional strengths and stiffnesses of carbon nanotubes. Physical Review B, 2005, 72, .	3.2	27
94	Equilibrium limits of coherency in strained nanowire heterostructures. Journal of Applied Physics, 2005, 97, 114325.	2.5	337
95	Equilibrium Analysis of Lattice-Mismatched Nanowire Heterostructures. Materials Research Society Symposia Proceedings, 2002, 737, 262.	0.1	8
96	Optical interconnects realizable with thinâ€“film helicoidal bianisotropic mediums. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2001, 457, 817-836.	2.1	6
97	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.	1.4	6
98	Toward Zero-Strain Mixed Conductors: Anomalously Low Redox Coefficients of Chemical Expansion in Praseodymium-Oxide Perovskites. Chemistry of Materials, 0, , .	6.7	3
99	Controlling thermoelectric transport via native defects in the diamond-like semiconductors Cu2HgGeTe4 and Hg2GeTe4. Journal of Materials Chemistry A, 0, , .	10.3	4