Elif Ertekin

List of Publications by Year in Descending Order

89 papers	2,873 citations	25 h-index	52 g-index
107 ext. papers	3,507 ext. citations	8.6 avg, IF	5.69 L-index

#	Paper	IF	Citations
89	Tuning valley degeneracy with band inversion. *Journal of Materials Chemistry A*, **2022**, 10, 1588-1595	13	0
88	Achieving a Carbon Neutral Future through Advanced Functional Materials and Technologies. *Bulletin of the Chemical Society of Japan*, **2022**, 95, 73-103	5.1	3
87	Multisublattice cluster expansion study of short-range ordering in iron-substituted strontium titanate. *Computational Materials Science*, **2022**, 202, 110969	3.2	
86	Pathways to controlled 3D deformation of graphene: Manipulating the motion of topological defects. *Current Opinion in Solid State and Materials Science*, **2021**, 25, 100893	12	2
85	Correlating Surface Crystal Orientation and Gas Kinetics in Perovskite Oxide Electrodes. *Advanced Materials*, **2021**, 33, e2100977	24	5
84	Native Defect Engineering in CuInTe2. *Chemistry of Materials*, **2021**, 33, 359-369	9.6	3
83	Designing the Bending Stiffness of 2D Material Heterostructures. *Advanced Materials*, **2021**, 33, e2007269	24	13
82	Mechanism of creation and destruction of oxygen interstitial atoms by nonpolar zinc oxide(101[combining macron]0) surfaces. *Physical Chemistry Chemical Physics*, **2021**, 23, 16423-16435	3.6	3
81	Tuning p-Si(111) Photovoltage via Molecule|Semiconductor Electronic Coupling. *Journal of the American Chemical Society*, **2021**, 143, 2567-2580	16.4	5
80	2D Materials: Designing the Bending Stiffness of 2D Material Heterostructures (Adv. Mater. 9/2021). *Advanced Materials*, **2021**, 33, 2170066	24	
79	Perovskite Na-ion conductors developed from analogous Li3xLa2/3□TiO3 (LLTO): chemo-mechanical and defect engineering. *Journal of Materials Chemistry A*, **2021**, 9, 21241-21258	13	0
78	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	9.6	12
77	Topologically derived dislocation theory for twist and stretch moiré superlattices in bilayer graphene. *Physical Review B*, **2020**, 102,	3.3	2
76	Material-Dependent Evolution of Mechanical Folding Instabilities in Two-Dimensional Atomic Membranes. *ACS Applied Materials & Interfaces*, **2020**, 12, 10801-10808	9.5	8
75	Stochastic Stress Jumps Due to Soliton Dynamics in Two-Dimensional van der Waals Interfaces. *Nano Letters*, **2020**, 20, 1201-1207	11.5	10
74	Ultrasoft slip-mediated bending in few-layer graphene. *Nature Materials*, **2020**, 19, 305-309	27	85
73	Designing Optimal Perovskite Structure for High Ionic Conduction. *Advanced Materials*, **2020**, 32, e1905128	24	17

72	Kinetic Control of Oxygen Interstitial Interaction with TiO(110) via the Surface Fermi Energy. *Langmuir*, **2020**, 36, 12632-12648	4	4
71	Toward design of cation transport in solid-state battery electrolytes: Structure-dynamics relationships. *Current Opinion in Solid State and Materials Science*, **2020**, 24, 100875	12	9
70	Fermi level dependence of gas-solid oxygen defect exchange mechanism on TiO (110) by first-principles calculations. *Journal of Chemical Physics*, **2020**, 153, 124710	3.9	3
69	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	5.6	3
68	Doping by design: finding new n-type dopable ABX4 Zintl phases for thermoelectrics. *Journal of Materials Chemistry A*, **2020**, 8, 25306-25315	13	5
67	Probing The Mechanical Properties of Few-Layer Graphene with Aberration-Corrected, Low-Voltage STEM. *Microscopy and Microanalysis*, **2019**, 25, 1730-1731	0.5	
66	Carrier density control in Cu2HgGeTe4 and discovery of Hg2GeTe4via phase boundary mapping. *Journal of Materials Chemistry A*, **2019**, 7, 621-631	13	16
65	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	35.4	31
64	Computational Approaches to Photoelectrode Design through Molecular Functionalization for Enhanced Photoelectrochemical Water Splitting. *ChemSusChem*, **2019**, 12, 1858-1871	8.3	6
63	Cluster Expansion Framework for the Sr(Ti1Fex)O3/2 (0 Chemistry of Materials, **2019**, 31, 3144-3153	9.6	3
62	Atomistic Mechanisms for the Thermal Relaxation of Au-hyperdoped Si. *Physical Review Applied*, **2019**, 12,	4.3	10
61	Asynchronous Photoexcited Electronic and Structural Relaxation in Lead-Free Perovskites. *Journal of the American Chemical Society*, **2019**, 141, 13074-13080	16.4	25
60	New kagome prototype materials: discovery of KV3Sb5,RbV3Sb5, and CsV3Sb5. *Physical Review Materials*, **2019**, 3,	3.2	101
59	Evidence for vacancy trapping in Au-hyperdoped Si following pulsed laser melting. *APL Materials*, **2019**, 7, 101124	5.7	8
58	Grain boundary structure and migration in graphene via the displacement shift complete lattice. *Acta Materialia*, **2019**, 166, 67-74	8.4	9
57	Origins and Control of Optical Absorption in a Nondilute Oxide Solid Solution: Sr(Ti,Fe)O3Perovskite Case Study. *Chemistry of Materials*, **2019**, 31, 1030-1041	9.6	12
56	Atomic Modeling and Electronic Structure of Mixed IonicElectronic Conductor SrTi1FexO3/2+Considered as a Mixture of SrTiO3 and Sr2Fe2O5. *Chemistry of Materials*, **2019**, 31, 233-243	9.6	11
55	Vibrational Energy Transport in Hybrid Ordered/Disordered Nanocomposites: Hybridization and Avoided Crossings of Localized and Delocalized Modes. *Advanced Functional Materials*, **2018**, 28, 1706268	15.6	17

54	Design Strategy for the Molecular Functionalization of Semiconductor Photoelectrodes: A Case Study of p-Si(111) Photocathodes for H Generation. *Langmuir*, **2018**, 34, 2959-2966	4	2
53	Multiscale Computational Design of Functionalized Photocathodes for H Generation. *Journal of the American Chemical Society*, **2018**, 140, 50-53	16.4	10
52	Ultralow Thermal Conductivity in Diamond-Like Semiconductors: Selective Scattering of Phonons from Antisite Defects. *Chemistry of Materials*, **2018**, 30, 3395-3409	9.6	16
51	Thermoelectric phonon-glass electron-crystal via ion beam patterning of silicon. *Physical Review B*, **2018**, 97,	3.3	16
50	Elastocaloric effects in the extreme. *Scripta Materialia*, **2018**, 148, 122-126	5.6	34
49	First-principles description of oxygen self-diffusion in rutile TiO: assessment of uncertainties due to enthalpy and entropy contributions. *Physical Chemistry Chemical Physics*, **2018**, 20, 17448-17457	3.6	10
48	Atomically precise graphene etch stops for three dimensional integrated systems from two dimensional material heterostructures. *Nature Communications*, **2018**, 9, 3988	17.4	33
47	Identifying Charge Transfer Mechanisms across Semiconductor Heterostructures via Surface Dipole Modulation and Multiscale Modeling. *Journal of the American Chemical Society*, **2018**, 140, 13223-13232	16.4	14
46	Computational Analysis of the Interplay between Deep Level Traps and Perovskite Solar Cell Efficiency. *Journal of the American Chemical Society*, **2018**, 140, 15655-15660	16.4	12
45	A Cocatalyst that Stabilizes a Hydride Intermediate during Photocatalytic Hydrogen Evolution over a Rhodium-Doped TiO Nanosheet. *Angewandte Chemie - International Edition*, **2018**, 57, 9073-9077	16.4	48
44	Atomic scale origins of sub-band gap optical absorption in gold-hyperdoped silicon. *AIP Advances*, **2018**, 8, 055014	1.5	11
43	A Cocatalyst that Stabilizes a Hydride Intermediate during Photocatalytic Hydrogen Evolution over a Rhodium-Doped TiO2 Nanosheet. *Angewandte Chemie*, **2018**, 130, 9211-9215	3.6	10
42	Asymmetric response of ferroelectric/metal oxide heterojunctions for catalysis arising from interfacial chemistry. *Physical Chemistry Chemical Physics*, **2017**, 19, 5870-5879	3.6	7
41	Fixed-node diffusion Monte Carlo description of nitrogen defects in zinc oxide. *Physical Review B*, **2017**, 95,	3.3	18
40	Plastic deformation of B2-NiTi is it slip or twinning?. *Philosophical Magazine Letters*, **2017**, 97, 217-228	1	25
39	Effect of Surface Coverage and Composition on the Stability and Interfacial Dipole of Functionalized Silicon. *Journal of Physical Chemistry C*, **2017**, 121, 11312-11318	3.8	12
38	Elastocaloric cooling capacity of shape memory alloys Role of deformation temperatures, mechanical cycling, stress hysteresis and inhomogeneity of transformation. *Acta Materialia*, **2017**, 135, 158-176	8.4	106
37	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	3.8	11

36	Computational insights into charge transfer across functionalized semiconductor surfaces. *Science and Technology of Advanced Materials*, **2017**, 18, 681-692	7.1	11
35	Structural and thermal effects of ion-irradiation induced defect configurations in silicon. *Physical Review B*, **2017**, 95,	3.3	8
34	First-Principle Study of the Electronic Structure and Stability of Reconstructed AgInSe2 (112) Polar Surfaces. *IEEE Journal of Photovoltaics*, **2017**, 7, 1781-1788	3.7	2
33	Screened-exchange density functional theory description of the electronic structure and phase stability of the chalcopyrite materials AgInSe2 and AuInSe2. *Physical Review B*, **2016**, 93,	3.3	5
32	Generalized Debye-Peierls/Allen-Feldman model for the lattice thermal conductivity of low-dimensional and disordered materials. *Physical Review B*, **2016**, 93,	3.3	54
31	Phonons, Localization, and Thermal Conductivity of Diamond Nanothreads and Amorphous Graphene. *Nano Letters*, **2016**, 16, 4763-72	11.5	121
30	Surface-assisted defect engineering of point defects in ZnO. *Applied Physics Letters*, **2016**, 108, 241603	3.4	22
29	Reducing extrinsic damping of surface acoustic waves at gigahertz frequencies. *Journal of Applied Physics*, **2016**, 119, 164301	2.5	4
28	Mechanism and energetics of O and O2 adsorption on polar and non-polar ZnO surfaces. *Journal of Chemical Physics*, **2016**, 144, 184708	3.9	19
27	Resolving anomalous strain effects on two-dimensional phonon flows: The cases of graphene, boron nitride, and planar superlattices. *Physical Review B*, **2015**, 91,	3.3	77
26	Elastocaloric cooling potential of NiTi, Ni2FeGa, and CoNiAl. *Acta Materialia*, **2015**, 96, 420-427	8.4	105
25	A novel, layered phase in Ti-rich SrTiO3 epitaxial thin films. *Advanced Materials*, **2015**, 27, 861-8	24	6
24	Photocatalytic reaction centers in two-dimensional titanium oxide crystals. *Journal of the American Chemical Society*, **2015**, 137, 239-44	16.4	125
23	Infrared thermography videos of the elastocaloric effect for shape memory alloys NiTi and Ni2FeGa. *Data in Brief*, **2015**, 5, 7-8	1.2	1
22	Phase stability and properties of manganese oxide polymorphs: Assessment and insights from diffusion Monte Carlo. *Physical Review B*, **2015**, 92,	3.3	30
21	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	3.9	33
20	Lattice mismatch induced ripples and wrinkles in planar graphene/boron nitride superlattices. *Journal of Applied Physics*, **2015**, 117, 234304	2.5	11
19	Ripples, strain, and misfit dislocations: structure of graphene-boron nitride superlattice interfaces. *Nano Letters*, **2015**, 15, 1468-75	11.5	38

18	Phonon transport on two-dimensional graphene/boron nitride superlattices. *Physical Review B*, **2014**, 90,	3.3	140
17	Extended X-ray absorption fine structure spectroscopy of selenium-hyperdoped silicon. *Journal of Applied Physics*, **2013**, 114, 133507	2.5	21
16	Point-defect optical transitions and thermal ionization energies from quantum Monte Carlo methods: Application to the F-center defect in MgO. *Physical Review B*, **2013**, 87,	3.3	41
15	Insulator-to-metal transition in selenium-hyperdoped silicon: observation and origin. *Physical Review Letters*, **2012**, 108, 026401	7.4	115
14	Interplay between intrinsic defects, doping, and free carrier concentration in SrTiO3 thin films. *Physical Review B*, **2012**, 85,	3.3	42
13	Interplay of wetting and elasticity in the nucleation of carbon nanotubes. *Physical Review Letters*, **2011**, 107, 185503	7.4	16
12	Plasticity in carbon nanotubes: Cooperative conservative dislocation motion. *Physical Review B*, **2010**, 81,	3.3	17
11	Superelastic metal-insulator phase transition in single-crystal VO2 nanobeams. *Physical Review B*, **2009**, 80,	3.3	33
10	Facets of nanotube synthesis: High-resolution transmission electron microscopy study and density functional theory calculations. *Physical Review B*, **2009**, 79,	3.3	25
9	Strain engineering and one-dimensional organization of metal-insulator domains in single-crystal vanadium dioxide beams. *Nature Nanotechnology*, **2009**, 4, 732-7	28.7	480
8	Topological description of the Stone-Wales defect formation energy in carbon nanotubes and graphene. *Physical Review B*, **2009**, 79,	3.3	70
7	Elasticity theory of topological defects in carbon nanotubes and graphene. *Philosophical Magazine Letters*, **2008**, 88, 159-167	1	7
6	Ideal torsional strengths and stiffnesses of carbon nanotubes. *Physical Review B*, **2005**, 72,	3.3	25
5	Equilibrium limits of coherency in strained nanowire heterostructures. *Journal of Applied Physics*, **2005**, 97, 114325	2.5	301
4	Equilibrium Analysis of Lattice-Mismatched Nanowire Heterostructures. *Materials Research Society Symposia Proceedings*, **2002**, 737, 262		5
3	Optical interconnects realizable with thin-film helicoidal bianisotropic mediums. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, **2001**, 457, 817-836	2.4	6
2	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	1.2	6
1	Toward Zero-Strain Mixed Conductors: Anomalously Low Redox Coefficients of Chemical Expansion in Praseodymium-Oxide Perovskites. *Chemistry of Materials*,	9.6	2