Alexander Chroneos

List of Publications by Citations

318 papers	7,086 citations	49 h-index	66 g-index
331 ext. papers	7,994 ext. citations	3.5 avg, IF	6.55 L-index

#	Paper	IF	Citations
318	Oxygen diffusion in solid oxide fuel cell cathode and electrolyte materials: mechanistic insights from atomistic simulations. *Energy and Environmental Science*, **2011**, 4, 2774	35.4	300
317	Anisotropic oxygen diffusion in tetragonal La2NiO4+ molecular dynamics calculations. *Journal of Materials Chemistry*, **2010**, 20, 266-270		161
316	Diffusion of n-type dopants in germanium. *Applied Physics Reviews*, **2014**, 1, 011301	17.3	128
315	Oxygen ion diffusion in cation ordered/disordered GdBaCo2O5+ *Journal of Materials Chemistry*, **2011**, 21, 2183-2186		128
314	Vacancy-mediated dopant diffusion activation enthalpies for germanium. *Applied Physics Letters*, **2008**, 92, 172103	3.4	123
313	Oxygen transport in perovskite and related oxides: A brief review. *Journal of Alloys and Compounds*, **2010**, 494, 190-195	5.7	114
312	Effect of strain on the oxygen diffusion in yttria and gadolinia co-doped ceria. *Solid State Ionics*, **2013**, 230, 37-42	3.3	94
311	Interstitialcy diffusion of oxygen in tetragonal La2CoO(4+). *Physical Chemistry Chemical Physics*, **2011**, 13, 2242-9	3.6	90
310	Elastic and thermodynamic properties of new (Zr3 Tix)AlC2 MAX-phase solid solutions. *Computational Materials Science*, **2017**, 137, 318-326	3.2	87
309	Impact of uniaxial strain and doping on oxygen diffusion in CeO2. *Scientific Reports*, **2014**, 4, 6068	4.9	85
308	Molecular dynamics study of oxygen diffusion in Pr(2)NiO(4+delta). *Physical Chemistry Chemical Physics*, **2010**, 12, 6834-6	3.6	82
307	Synthesis and DFT investigation of new bismuth-containing MAX phases. *Scientific Reports*, **2016**, 6, 18829	4.9	82
306	Anisotropic oxygen diffusion in PrBaCo2O5.5 double perovskites. *Solid State Ionics*, **2012**, 216, 41-43	3.3	77
305	Diffusion and defect reactions between donors, C, and vacancies in Ge. II. Atomistic calculations of related complexes. *Physical Review B*, **2008**, 77,	3.3	75
304	Deviations from Vegard s law in ternary III-V alloys. *Physical Review B*, **2010**, 82,	3.3	74
303	Diffusion of E centers in germanium predicted using GGA+U approach. *Applied Physics Letters*, **2011**, 99, 072112	3.4	73
302	Genetics of superionic conductivity in lithium lanthanum titanates. *Physical Chemistry Chemical Physics*, **2015**, 17, 178-83	3.6	72

301	Vacancy-arsenic clusters in germanium. *Applied Physics Letters*, **2007**, 91, 192106	3.4	70
300	Carbon, dopant, and vacancy interactions in germanium. *Journal of Applied Physics*, **2007**, 102, 083707	2.5	68
299	Fluorine effect on As diffusion in Ge. *Journal of Applied Physics*, **2011**, 109, 113527	2.5	65
298	Modeling self-diffusion in UO2 and ThO2 by connecting point defect parameters with bulk properties. *Solid State Ionics*, **2015**, 274, 1-3	3.3	64
297	S-functionalized MXenes as electrode materials for Li-ion batteries. *Applied Materials Today*, **2016**, 5, 19-24	6.6	64
296	Intrinsic and extrinsic diffusion of indium in germanium. *Journal of Applied Physics*, **2009**, 106, 063534	2.5	63
295	Oxygen diffusion in Sr0.75Y0.25CoO2.625: A molecular dynamics study. *Physical Review B*, **2009**, 79,	3.3	63
294	c-axis hopping conductivity in heavily Pr-doped YBCO single crystals. *Superconductor Science and Technology*, **2013**, 26, 085017	3.1	62
293	Point defect engineering strategies to suppress A-center formation in silicon. *Applied Physics Letters*, **2011**, 99, 241901	3.4	62
292	Defect processes in orthorhombic LnBaCo2O5.5 double perovskites. *Physical Chemistry Chemical Physics*, **2011**, 13, 15305-10	3.6	61
291	Strain-induced changes to the electronic structure of germanium. *Journal of Physics Condensed Matter*, **2012**, 24, 195802	1.8	58
290	Fluctuation conductivity and pseudogap in single crystals under pressure with transport current flowing under an angle 45□to the twin boundaries. *Physica C: Superconductivity and Its Applications*, **2014**, 501, 24-31	1.3	57
289	Defect interactions in Sn1⊠Gex random alloys. *Applied Physics Letters*, **2009**, 94, 252104	3.4	57
288	Detecting anomalies in time series data via a deep learning algorithm combining wavelets, neural networks and Hilbert transform. *Expert Systems With Applications*, **2017**, 85, 292-304	7.8	56
287	Impact of isovalent doping on the trapping of vacancy and interstitial related defects in Si. *Journal of Applied Physics*, **2013**, 113, 113506	2.5	56
286	Electro-transport and structure of 1-2-3 HTSC single crystals with different plane defects topologies. *Journal of Materials Science: Materials in Electronics*, **2012**, 23, 1255-1259	2.1	56
285	Oxygen defect processes in silicon and silicon germanium. *Applied Physics Reviews*, **2015**, 2, 021306	17.3	55
284	Effect of tin doping on oxygen- and carbon-related defects in Czochralski silicon. *Journal of Applied Physics*, **2011**, 110, 093507	2.5	55

283	Nonlinear stability of E centers in Si1−xGex: Electronic structure calculations. *Physical Review B*, **2008**, 78,	3.3	55
282	Attempts to synthesise quaternary MAX phases (Zr,M)2AlC and Zr2(Al,A)C as a way to approach Zr2AlC. *Materials Research Letters*, **2016**, 4, 137-144	7.4	54
281	Interaction of A-centers with isovalent impurities in silicon. *Journal of Applied Physics*, **2010**, 107, 093518	2.5	54
280	Phase separation in oxygen deficient Ba2Cu3O7-δ single crystals: effect of high pressure and twin boundaries. *Philosophical Magazine*, **2011**, 91, 2291-2302	1.6	54
279	Fluorine codoping in germanium to suppress donor diffusion and deactivation. *Journal of Applied Physics*, **2009**, 106, 063707	2.5	52
278	The Effect of Ion Size on Solution Mechanism and Defect Cluster Geometry. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1997**, 101, 1204-1210		52
277	Effect of high pressure on the fluctuation conductivity and the charge transfer of YBa2Cu3O7−δ single crystals. *Journal of Alloys and Compounds*, **2008**, 453, 69-74	5.7	52
276	Implantation and diffusion of phosphorous in germanium. *Materials Science in Semiconductor Processing*, **2006**, 9, 640-643	4.3	50
275	Synthesis and physical properties of (Zr1−x,Tix)3AlC2 MAX phases. *Journal of the American Ceramic Society*, **2017**, 100, 3393-3401	3.8	49
274	Structural relaxation, metal-to-insulator transition and pseudo-gap in oxygen deficient Ba2Cu3O7−δ single crystals. *Physica C: Superconductivity and Its Applications*, **2009**, 469, 203-206	1.3	49
273	E centers in ternary Si1−x−yGexSny random alloys. *Applied Physics Letters*, **2009**, 95, 112101	3.4	49
272	Review of Recent Studies on Solution Combustion Synthesis of Nanostructured Catalysts. *Advanced Engineering Materials*, **2018**, 20, 1800047	3.5	48
271	Impact of germanium on vacancy clustering in germanium-doped silicon. *Journal of Applied Physics*, **2009**, 105, 016102	2.5	47
270	Isovalent impurity-vacancy complexes in germanium. *Physica Status Solidi (B): Basic Research*, **2007**, 244, 3206-3210	1.3	47
269	Phosphorous clustering in germanium-rich silicon germanium. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2008**, 154-155, 72-75	3.1	47
268	Physical properties of the recently discovered Zr2(Al1− x Bi x)C MAX phases. *Journal of Materials Science: Materials in Electronics*, **2016**, 27, 11925-11933	2.1	45
267	Fluctuation conductivity of oxygen underdoped YBa2Cu3O7−δ single crystals. *Physica B: Condensed Matter*, **2014**, 436, 88-90	2.8	45
266	The thermodynamics of hydride precipitation: The importance of entropy, enthalpy and disorder. *Acta Materialia*, **2014**, 79, 351-362	8.4	45

265	Defects, dopants and Mg diffusion in MgTiO. *Scientific Reports*, **2019**, 9, 4394	4.9	44
264	INFLUENCE OF HIGH PRESSURE ON THE TEMPERATURE-DEPENDENCE OF THE PSEUDO-GAP IN OXYGEN DEFICIENT YBa2Cu3O7-δ SINGLE CRYSTALS. *Modern Physics Letters B*, **2010**, 24, 2295-2301	1.6	44
263	Intrinsic Defects and H Doping in WO. *Scientific Reports*, **2017**, 7, 40882	4.9	43
262	Effect of praseodymium on the electrical resistance of $Y_{2}Ba_{4}Cu_{7}O_{15}$ single crystals. *Solid State Communications*, **2014**, 190, 18-22	1.6	43
261	Metal-to-insulator transition in $Y_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$ single crystals with various praseodymium contents. *Physica C: Superconductivity and Its Applications*, **2013**, 485, 89-91	1.3	43
260	INFLUENCE OF LONGITUDINAL MAGNETIC FIELD ON THE FLUCTUATION CONDUCTIVITY IN SLIGHTLY Al-DOPED YBa2Cu3-zAlzO7-δ SINGLE CRYSTALS WITH A GIVEN TOPOLOGY OF PLANE DEFECTS. *Modern Physics Letters B*, **2011**, 25, 2131-2136	1.6	43
259	Modeling oxygen self-diffusion in UO2 under pressure. *Solid State Ionics*, **2015**, 282, 26-30	3.3	42
258	Effect of long aging on the resistivity properties of optimally doped $YBa_2Cu_3O_{7-\delta}$ single crystals. *Solid State Communications*, **2013**, 170, 6-9	1.6	42
257	Effect of annealing on a pseudogap state in untwinned YBaCuO single crystals. *Scientific Reports*, **2019**, 9, 9274	4.9	41
256	Nb-based MXenes for Li-ion battery applications. *Physica Status Solidi - Rapid Research Letters*, **2015**, 9, 726-729	2.5	41
255	Relaxation of the normal electrical resistivity induced by high-pressure in strongly underdoped $YBa_2Cu_3O_{7-\delta}$ single crystals. *Physica B: Condensed Matter*, **2012**, 407, 4470-4472	2.8	40
254	Transport anisotropy and pseudo-gap state in oxygen deficient $ReBa_2Cu_3O_{7-\delta}$ (Re=Y, Ho) single crystals. *Journal of Alloys and Compounds*, **2008**, 464, 58-66	5.7	39
253	Effect of small oxygen deficiency on the para-coherent transition and 2D–3D crossover in untwinned $YBa_2Cu_3O_{7-\delta}$ single crystals. *Journal of Alloys and Compounds*, **2011**, 509, 4553-4556	5.7	38
252	Effect of high pressure on the metal-dielectric transition and the pseudo-gap temperature range in oxygen deficient $YBa_2Cu_3O_{7-\delta}$ single crystals. *Journal of Materials Science: Materials in Electronics*, **2011**, 22, 20-24	2.1	38
251	Evolution of the Fishtail-Effect in Pure and Ag-doped MG-YBCO. *Journal of Low Temperature Physics* , **2010**, 161, 387-394	1.3	38
250	Excess conductivity and pseudo-gap state in YBCO single crystals slightly doped with Al and Pr. *Journal of Materials Science: Materials in Electronics*, **2007**, 18, 811-815	2.1	38
249	Vacancies and defect levels in III–V semiconductors. *Journal of Applied Physics*, **2013**, 114, 063517	2.5	37
248	Nuclear wasteform materials: Atomistic simulation case studies. *Journal of Nuclear Materials*, **2013**, 441, 29-39	3.3	37

247	Silicene/germanene on MgX2 (X = Cl, Br, and I) for Li-ion battery applications. *Nanoscale*, **2016**, 8, 7272-7	7.7	36
246	A-centers in silicon studied with hybrid density functional theory. *Applied Physics Letters*, **2013**, 103, 052101	3.4	36
245	Resistive investigation of pseudogap state in non-stoichiometric ReBa2Cu3O7−δ (Re = Y, Ho) single crystals with account for BCS–BEC crossover. *Journal of Alloys and Compounds*, **2009**, 485, L21-L23	5.7	36
244	Defect process and lithium diffusion in Li2TiO3. *Solid State Ionics*, **2018**, 327, 93-98	3.3	35
243	Effect of high pressure on the electrical resistivity of optimally doped YBa2Cu3O7−δ single crystals with unidirectional planar defects. *Physica B: Condensed Matter*, **2013**, 422, 33-35	2.8	34
242	Carbon related defects in irradiated silicon revisited. *Scientific Reports*, **2014**, 4, 4909	4.9	34
241	Experimental synthesis and density functional theory investigation of radiation tolerance of Zr3(Al1-xSix)C2 MAX phases. *Journal of the American Ceramic Society*, **2017**, 100, 1377-1387	3.8	33
240	Physical properties and defect processes of M3SnC2 (M = Ti, Zr, Hf) MAX phases: Effect of M-elements. *Journal of Alloys and Compounds*, **2018**, 748, 804-813	5.7	33
239	Atomic scale simulations of arsenic–vacancy complexes in germanium and silicon. *Materials Science in Semiconductor Processing*, **2006**, 9, 536-540	4.3	33
238	Defect chemistry of doped bixbyite oxides. *Solid State Sciences*, **2007**, 9, 588-593	3.4	32
237	Lithium Doping of ZnO for High Efficiency and Stability Fullerene and Non-fullerene Organic Solar Cells. *ACS Applied Energy Materials*, **2019**, 2, 1663-1675	6.1	30
236	A perspective on MXenes: Their synthesis, properties, and recent applications. *Journal of Applied Physics*, **2020**, 128, 170902	2.5	30
235	Defects and dopant properties of LiV(PO). *Scientific Reports*, **2019**, 9, 333	4.9	29
234	Defects, Dopants and Sodium Mobility in NaMnSiO. *Scientific Reports*, **2018**, 8, 14669	4.9	29
233	Lithium diffusion in LiFeO. *Scientific Reports*, **2018**, 8, 5832	4.9	28
232	LiSnO as a Cathode Material for Lithium-ion Batteries: Defects, Lithium Ion Diffusion and Dopants. *Scientific Reports*, **2018**, 8, 12621	4.9	28
231	Defect Chemistry and Li-ion Diffusion in LiRuO. *Scientific Reports*, **2019**, 9, 550	4.9	27
230	Intrinsic defect processes and elastic properties of Ti3AC2 (A = Al, Si, Ga, Ge, In, Sn) MAX phases. *Journal of Applied Physics*, **2018**, 123, 025103	2.5	27

229	Peculiarities of pseudogap in YPrBaCuO single crystals under pressure up to 1.7 GPa. *Scientific Reports*, **2019**, 9, 20424	4.9	27
228	Defects and lithium migration in LiCuO. *Scientific Reports*, **2018**, 8, 6754	4.9	26
227	Impurity diffusion, point defect engineering, and surface/interface passivation in germanium. *Annalen Der Physik*, **2012**, 524, 123-132	2.6	26
226	Diffusion of tin in germanium: A GGA+U approach. *Applied Physics Letters*, **2011**, 99, 162103	3.4	26
225	Engineering the free vacancy and active donor concentrations in phosphorus and arsenic double donor-doped germanium. *Journal of Applied Physics*, **2008**, 104, 113724	2.5	26
224	Defects, dopants and Li-ion diffusion in Li2SiO3. *Solid State Ionics*, **2019**, 335, 61-66	3.3	25
223	Point defect engineering strategies to retard phosphorous diffusion in germanium. *Physical Chemistry Chemical Physics*, **2013**, 15, 367-71	3.6	23
222	New atomic scale simulation models for hydroxides and oxyhydroxides. *Journal of Materials Science* , **2006**, 41, 675-687	4.3	23
221	Connecting point defect parameters with bulk properties to describe diffusion in solids. *Applied Physics Reviews*, **2016**, 3, 041304	17.3	23
220	Learning Driver Braking Behavior Using Smartphones, Neural Networks and the Sliding Correlation Coefficient: Road Anomaly Case Study. *IEEE Transactions on Intelligent Transportation Systems*, **2019** , 20, 65-74	6.1	23
219	Solution combustion synthesis of nano-catalysts with a hierarchical structure. *Journal of Catalysis*, **2018**, 364, 112-124	7.3	23
218	A-centers and isovalent impurities in germanium: Density functional theory calculations. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2011**, 176, 453-457	3.1	22
217	Concentration of intrinsic defects and self-diffusion in GaSb. *Journal of Applied Physics*, **2008**, 104, 093714	2.5	22
216	A thermodynamic approach of self- and hetero-diffusion in GaAs: connecting point defect parameters with bulk properties. *RSC Advances*, **2016**, 6, 53324-53330	3.7	22
215	Phase stability and the arsenic vacancy defect in InxGa1−xAs. *Physical Review B*, **2011**, 84,	3.3	21
214	Defects, Lithium Mobility and Tetravalent Dopants in the LiNbO Cathode Material. *Scientific Reports*, **2019**, 9, 2192	4.9	21
213	Defects, Dopants and Lithium Mobility in Li V (P O) (PO). *Scientific Reports*, **2018**, 8, 8140	4.9	21
212	Composition and temperature dependence of self-diffusion in Si Ge alloys. *Scientific Reports*, **2017**, 7, 1374	4.9	20

211	Impact of doping on the ionic conductivity of ceria: a comprehensive model. *Journal of Chemical Physics*, **2013**, 138, 224705	3.9	20
210	Formation and evolution of oxygen-vacancy clusters in lead and tin doped silicon. *Journal of Applied Physics*, **2012**, 111, 123508	2.5	20
209	Li3SbO4 lithium-ion battery material: Defects, lithium ion diffusion and tetravalent dopants. *Materials Chemistry and Physics*, **2019**, 225, 34-41	4.4	20
208	Influence of planar and point defects on the basal-plane conductivity of HoBaCuO single crystals. *Physica C: Superconductivity and Its Applications*, **2015**, 516, 58-61	1.3	19
207	Modelling zirconium hydrides using the special quasirandom structure approach. *Physical Chemistry Chemical Physics*, **2013**, 15, 7599-603	3.6	19
206	Structural and optical properties of the recently synthesized (Zr3 Ti x)AlC2 MAX phases. *Journal of Materials Science: Materials in Electronics*, **2017**, 28, 3386-3393	2.1	19
205	Atomic scale simulations of donor acancy pairs in germanium. *Journal of Materials Science: Materials in Electronics*, **2007**, 18, 763-768	2.1	19
204	A roadmap of strain in doped anatase TiO. *Scientific Reports*, **2018**, 8, 12790	4.9	18
203	Hydrogen and nitrogen codoping of anatase TiO for efficiency enhancement in organic solar cells. *Scientific Reports*, **2017**, 7, 17839	4.9	18
202	Effect of carbon on dopant acancy pair stability in germanium. *Semiconductor Science and Technology*, **2011**, 26, 095017	1.8	18
201	Defect processes in F and Cl doped anatase TiO. *Scientific Reports*, **2019**, 9, 19970	4.9	18
200	A thermodynamic approach to self-diffusion in silicon: Evidence of a single diffusion mechanism?. *Materials Chemistry and Physics*, **2016**, 181, 204-208	4.4	17
199	Modification of superconducting and resistive properties of HoBa2Cu3O7 single crystals under application-removal of high hydrostatic pressure. *Modern Physics Letters B*, **2016**, 30, 1650188	1.6	16
198	Optimized hydrogen positions for aluminium and iron containing hydroxide minerals. *Journal of Materials Science*, **2007**, 42, 2024-2029	4.3	16
197	Engineering Transport in Manganites by Tuning Local Nonstoichiometry in Grain Boundaries. *Advanced Materials*, **2019**, 31, e1805360	24	16
196	Influence of atomic structure on the nano-nickel-based catalyst activity produced by solution combustion synthesis in the hydrogenation of maleic acid. *Journal of Catalysis*, **2017**, 348, 9-21	7.3	15
195	Modelling solid solutions with cluster expansion, special quasirandom structures, and thermodynamic approaches. *Applied Physics Reviews*, **2017**, 4, 041301	17.3	15
194	Na3V(PO4)2 cathode material for Na ion batteries: Defects, dopants and Na diffusion. *Solid State Ionics*, **2019**, 336, 75-79	3.3	15

193	Vacancy-oxygen defects in silicon: the impact of isovalent doping. *Journal of Materials Science: Materials in Electronics*, **2014**, 25, 2395-2410	2.1	15
192	Diffusion in energy materials: Governing dynamics from atomistic modelling. *Applied Physics Reviews*, **2017**, 4, 031305	17.3	15
191	Special quasirandom structures for gadolinia-doped ceria and related materials. *Physical Chemistry Chemical Physics*, **2012**, 14, 11737-42	3.6	15
190	A high-entropy manganite in an ordered nanocomposite for long-term application in solid oxide cells. *Nature Communications*, **2021**, 12, 2660	17.4	15
189	Different diffusion mechanisms of oxygen in ReBa 2 Cu 3 O 7 (Re = Y, Ho) single crystals. *Physica C: Superconductivity and Its Applications*, **2017**, 536, 26-29	1.3	14
188	Fluctuation conductivity and possible pseudogap state in FeAs-based superconductor EuFeAsO0.85F0.15. *Materials Research Express*, **2016**, 3, 076001	1.7	14
187	Doping strategies to control A-centres in silicon: insights from hybrid density functional theory. *Physical Chemistry Chemical Physics*, **2014**, 16, 8487-92	3.6	14
186	Modeling indium diffusion in germanium by connecting point defect parameters with bulk properties. *Journal of Materials Science: Materials in Electronics*, **2015**, 26, 2113-2116	2.1	14
185	Defect configurations of high-k cations in germanium. *Journal of Applied Physics*, **2012**, 111, 023714	2.5	14
184	Unexpected relationship between interlayer distances and surface/cleavage energies in TiAl: density functional study. *Journal of Physics Condensed Matter*, **2011**, 23, 265009	1.8	14
183	Carbon, oxygen and intrinsic defect interactions in germanium-doped silicon. *Semiconductor Science and Technology*, **2011**, 26, 105024	1.8	14
182	Describing oxygen self-diffusion in PuO2 by connecting point defect parameters with bulk properties. *Journal of Materials Science: Materials in Electronics*, **2015**, 26, 3287-3290	2.1	13
181	Connecting bulk properties of germanium with the behavior of self- and dopant diffusion. *Materials Science in Semiconductor Processing*, **2015**, 36, 179-183	4.3	13
180	Defect engineering of the oxygen-vacancy clusters formation in electron irradiated silicon by isovalent doping: An infrared perspective. *Journal of Applied Physics*, **2012**, 112, 123517	2.5	13
179	LOCALIZATION EFFECT AND PSEUDOGAP IN PRASEODYMIUM DOPED Y1-zPrzBa2Cu3O7- SINGLE CRYSTALS. *Modern Physics Letters B*, **2012**, 26, 1250163	1.6	13
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177	312 MAX Phases: Elastic Properties and Lithiation. *Materials*, **2019**, 12,	3.5	13
176	Insights into the physical properties of a new 211 MAX phase Nb2CuC. *Journal of Physics and Chemistry of Solids*, **2021**, 149, 109759	3.9	13

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174	Defect Chemistry and Na-Ion Diffusion in NaFe(PO) Cathode Material. *Materials*, **2019**, 12,	3.5	12
173	Chemically stable new MAX phase VSnC: a damage and radiation tolerant TBC material.. *RSC Advances*, **2020**, 10, 43783-43798	3.7	12
172	The encapsulation selectivity for anionic fission products imparted by an electride. *Scientific Reports*, **2019**, 9, 13612	4.9	12
171	Ultrafast palladium diffusion in germanium. *Journal of Materials Chemistry A*, **2015**, 3, 3832-3838	13	12
170	Defect engineering strategies for germanium. *Journal of Materials Science: Materials in Electronics*, **2013**, 24, 1741-1747	2.1	12
169	Extrinsic doping in silicon revisited. *Applied Physics Letters*, **2010**, 96, 242107	3.4	12
168	Toward Defect Engineering Strategies to Optimize Energy and Electronic Materials. *Applied Sciences (Switzerland)*, **2017**, 7, 674	2.6	11
167	G-centers in irradiated silicon revisited: A screened hybrid density functional theory approach. *Journal of Applied Physics*, **2014**, 115, 183509	2.5	11
166	Interaction of oxygen vacancies in yttrium germanates. *Physical Chemistry Chemical Physics*, **2012**, 14, 14630-4	3.6	11
165	Production and evolution of A-centers in n-type Si1−xGex. *Journal of Applied Physics*, **2013**, 113, 113507	2.5	11
164	Special quasirandom structures for binary/ternary group IV random alloys. *Chemical Physics Letters*, **2010**, 493, 97-102	2.5	11
163	Thermodynamic calculations of oxygen self-diffusion in mixed-oxide nuclear fuels. *RSC Advances*, **2016**, 6, 74018-74027	3.7	11
162	Defects, Diffusion, and Dopants in LiTiO: Atomistic Simulation Study. *Materials*, **2019**, 12,	3.5	10
161	Defect Process, Dopant Behaviour and Li Ion Mobility in the Li2MnO3 Cathode Material. *Energies*, **2019**, 12, 1329	3.1	10
160	Copper diffusion in germanium: connecting point defect parameters with bulk properties. *Journal of Materials Science: Materials in Electronics*, **2015**, 26, 2693-2696	2.1	10
159	Antisites and anisotropic diffusion in GaAs and GaSb. *Applied Physics Letters*, **2013**, 103, 142107	3.4	10
158	Impact of isovalent doping on radiation defects in silicon. *Journal of Applied Physics*, **2013**, 114, 113504	2.5	10

157	Co-doping with antimony to control phosphorous diffusion in germanium. *Journal of Applied Physics* , **2013**, 113, 073704	2.5	10
156	Ab initio modeling of MAX phase solid solutions using the special quasirandom structure approach. *Physical Chemistry Chemical Physics*, **2018**, 20, 1173-1180	3.6	10
155	Defect, Diffusion and Dopant Properties of NaNiO2: Atomistic Simulation Study. *Energies*, **2019**, 12, 3094	3.1	9
154	Technetium Encapsulation by A Nanoporous Complex Oxide 12CaO·7AlO (C12A7). *Nanomaterials*, **2019**, 9,	5.4	9
153	Effect of trivalent dopants on local coordination and electronic structure in crystalline and amorphous ZnO. *Thin Solid Films*, **2014**, 555, 117-121	2.2	9
152	Phosphorous–vacancy–oxygen defects in silicon. *Journal of Materials Chemistry A*, **2013**, 1, 11384	13	9
151	Anomaly detection in time series data using a combination of wavelets, neural networks and Hilbert transform **2015**,		9
150	Mechanisms of nonstoichiometry in HfN1−x. *Journal of Applied Physics*, **2009**, 106, 083502	2.5	9
149	Interaction of n-type dopants with oxygen in silicon and germanium. *Journal of Applied Physics*, **2012**, 112, 073706	2.5	9
148	Palladium diffusion in germanium. *Journal of Materials Science: Materials in Electronics*, **2015**, 26, 3787-3789	2.8	8
147	Migration of sodium and lithium interstitials in anatase TiO2. *Solid State Ionics*, **2018**, 315, 40-43	3.3	8
146	Mg6MnO8 as a Magnesium-Ion Battery Material: Defects, Dopants and Mg-Ion Transport. *Energies*, **2019**, 12, 3213	3.1	8
145	Stress-enhanced lithiation in MAX compounds for battery applications. *Applied Materials Today*, **2017**, 9, 192-195	6.6	8
144	Impact of isovalent doping on the formation of the C i O i (Si I) n defects in silicon. *Solid State Communications*, **2017**, 263, 19-22	1.6	8
143	Antisites in III-V semiconductors: Density functional theory calculations. *Journal of Applied Physics*, **2014**, 116, 023505	2.5	8
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141	Diffusion and Dopant Activation in Germanium: Insights from Recent Experimental and Theoretical Results. *Applied Sciences (Switzerland)*, **2019**, 9, 2454	2.6	7
140	Germanium diffusion in aluminium: connection between point defect parameters with bulk properties. *Journal of Materials Science: Materials in Electronics*, **2015**, 26, 8421-8424	2.1	7

139	Effect of electron irradiation on the fluctuation conductivity in YBa2Cu3O7 single crystals. *Journal of Materials Science: Materials in Electronics*, **2018**, 29, 7725-7729	2.1	7
138	Probabilistic kernel machines for predictive monitoring of weld residual stress in energy systems. *Engineering Applications of Artificial Intelligence*, **2018**, 71, 138-154	7.2	7
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