

Alexander Chroneos

List of Publications by Year in descending order

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328
papers

8,838
citations

26630

56
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71685

76
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all docs

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331
times ranked

5546
citing authors

#	ARTICLE	IF	CITATIONS
1	Oxygen diffusion in solid oxide fuel cell cathode and electrolyte materials: mechanistic insights from atomistic simulations. <i>Energy and Environmental Science</i> , 2011, 4, 2774.	30.8	354
2	Anisotropic oxygen diffusion in tetragonal $\text{La}_{2}\text{NiO}_{4+\delta}$: molecular dynamics calculations. <i>Journal of Materials Chemistry</i> , 2010, 20, 266-270.	6.7	199
3	Diffusion of <i>n</i> -type dopants in germanium. <i>Applied Physics Reviews</i> , 2014, 1, 011301.	11.3	146
4	Oxygen ion diffusion in cation ordered/disordered $\text{GdBaCo}_{2}\text{O}_{5+\delta}$. <i>Journal of Materials Chemistry</i> , 2011, 21, 2183-2186.	6.7	139
5	Vacancy-mediated dopant diffusion activation enthalpies for germanium. <i>Applied Physics Letters</i> , 2008, 92, .	3.3	132
6	Oxygen transport in perovskite and related oxides: A brief review. <i>Journal of Alloys and Compounds</i> , 2010, 494, 190-195.	5.5	126
7	Elastic and thermodynamic properties of new $(\text{Zr}_{3}\text{Ti})\text{AlC}_{2}$ MAX-phase solid solutions. <i>Computational Materials Science</i> , 2017, 137, 318-326.	3.0	119
8	Effect of strain on the oxygen diffusion in yttria and gadolinia co-doped ceria. <i>Solid State Ionics</i> , 2013, 230, 37-42.	2.7	114
9	Impact of uniaxial strain and doping on oxygen diffusion in CeO_{2} . <i>Scientific Reports</i> , 2014, 4, 6068.	3.3	106
10	Interstitialcy diffusion of oxygen in tetragonal $\text{La}_{2}\text{CoO}_{4+\delta}$. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 2242-2249.	2.8	104
11	Synthesis and DFT investigation of new bismuth-containing MAX phases. <i>Scientific Reports</i> , 2016, 6, 18829.	3.3	97
12	Molecular dynamics study of oxygen diffusion in $\text{Pr}_{2}\text{NiO}_{4+\delta}$. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6834.	2.8	96
13	Anisotropic oxygen diffusion in $\text{PrBaCo}_{2}\text{O}_{5.5}$ double perovskites. <i>Solid State Ionics</i> , 2012, 216, 41-43.	2.7	92
14	Deviations from Vegard's law in ternary III-V alloys. <i>Physical Review B</i> , 2010, 82, .	3.2	89
15	S-functionalized MXenes as electrode materials for Li-ion batteries. <i>Applied Materials Today</i> , 2016, 5, 19-24.	4.3	89
16	Detecting anomalies in time series data via a deep learning algorithm combining wavelets, neural networks and Hilbert transform. <i>Expert Systems With Applications</i> , 2017, 85, 292-304.	7.6	86
17	Genetics of superionic conductivity in lithium lanthanum titanates. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 178-183.	2.8	85
18	Review of Recent Studies on Solution Combustion Synthesis of Nanostructured Catalysts. <i>Advanced Engineering Materials</i> , 2018, 20, 1800047.	3.5	85

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37	Intrinsic Defects and H Doping in WO ₃ . Scientific Reports, 2017, 7, 40882.	3.3	65
38	E centers in ternary Si _{1-x} Ge _x Sny random alloys. Applied Physics Letters, 2009, 95, .	3.3	64
39	Nonlinear stability of E centers in Si _{1-x} Ge _x Sny random alloys. Applied Physics Letters, 2009, 95, . Electronic structure calculations. Physical Review B, 2009, 79, .	3.2	63
40	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.	1.2	63
41	Synthesis and physical properties of (Zr _{1-x} Ti _x) ₃ AlC ₂ MAX phases. Journal of the American Ceramic Society, 2017, 100, 3393-3401.	3.8	63
42	Defects, dopants and Mg diffusion in MgTiO ₃ . Scientific Reports, 2019, 9, 4394.	3.3	63
43	Dopant-vacancy cluster formation in germanium. Journal of Applied Physics, 2010, 107, .	2.5	62
44	Fluorine codoping in germanium to suppress donor diffusion and deactivation. Journal of Applied Physics, 2009, 106, .	2.5	61
45	Phase separation in oxygen deficient Ba ₂ Cu ₃ O _{7-δ} single crystals: effect of high pressure and twin boundaries. Philosophical Magazine, 2011, 91, 2291-2302.	1.6	61
46	Impact of isovalent doping on the trapping of vacancy and interstitial related defects in Si. Journal of Applied Physics, 2013, 113, 113506.	2.5	61
47	Nb-based MXenes for Li-ion battery applications. Physica Status Solidi - Rapid Research Letters, 2015, 9, 726-729.	2.4	61
48	Silicene/germanene on MgX ₂ (X = Cl, Br, and I) for Li-ion battery applications. Nanoscale, 2016, 8, 7272-7277.	5.6	61
49	Implantation and diffusion of phosphorous in germanium. Materials Science in Semiconductor Processing, 2006, 9, 640-643.	4.0	59
50	Effect of high pressure on the fluctuation conductivity and the charge transfer of YBa ₂ Cu ₃ O _{7-δ} single crystals. Journal of Alloys and Compounds, 2008, 453, 69-74.	5.5	59
51	Effect of germanium substrate loss and nitrogen on dopant diffusion in germanium. Journal of Applied Physics, 2009, 105, .	2.5	59
52	Interaction of A-centers with isovalent impurities in silicon. Journal of Applied Physics, 2010, 107, 093518.	2.5	59
53	The thermodynamics of hydride precipitation: The importance of entropy, enthalpy and disorder. Acta Materialia, 2014, 79, 351-362.	7.9	59
54	The Effect of Ion Size on Solution Mechanism and Defect Cluster Geometry. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1997, 101, 1204-1210.	0.9	58

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55	The vacancy in silicon: A critical evaluation of experimental and theoretical results. Journal of Applied Physics, 2008, 104, 076108.	2.5	58
56	Effect of tin doping on oxygen- and carbon-related defects in Czochralski silicon. Journal of Applied Physics, 2011, 110, .	2.5	58
57	Effect of annealing on a pseudogap state in untwinned YBa ₂ Cu ₃ O _{7-δ} single crystals. Scientific Reports, 2019, 9, 9274.	3.3	57
58	Impact of germanium on vacancy clustering in germanium-doped silicon. Journal of Applied Physics, 2009, 105, .	2.5	56
59	Modeling oxygen self-diffusion in UO ₂ under pressure. Solid State Ionics, 2015, 282, 26-30.	2.7	55
60	Isovalent impurity-vacancy complexes in germanium. Physica Status Solidi (B): Basic Research, 2007, 244, 3206-3210.	1.5	54
61	Structural relaxation, metal-to-insulator transition and pseudo-gap in oxygen deficient $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ single crystals. Physica C: Superconductivity and Its Applications, 2009, 469, 203-206.	1.2	54
62	Effect of praseodymium on the electrical resistance of Y _{1-x} Pr _x Ba ₂ Cu ₃ O _{7-δ} single crystals. Solid State Communications, 2014, 190, 18-22.	1.9	54
63	Vacancies and defect levels in III-V semiconductors. Journal of Applied Physics, 2013, 114, .	2.5	53
64	Lithium Doping of ZnO for High Efficiency and Stability Fullerene and Non-fullerene Organic Solar Cells. ACS Applied Energy Materials, 2019, 2, 1663-1675.	5.1	52
65	Phosphorous clustering in germanium-rich silicon germanium. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2008, 154-155, 72-75.	3.5	51
66	Physical properties and defect processes of M ₃ SnC ₂ (M= Ti, Zr, Hf) MAX phases: Effect of M-elements. Journal of Alloys and Compounds, 2018, 748, 804-813.	5.5	49
67	INFLUENCE OF HIGH PRESSURE ON THE TEMPERATURE-DEPENDENCE OF THE PSEUDO-GAP IN OXYGEN DEFICIENT YBa ₂ Cu ₃ O _{7-δ} SINGLE CRYSTALS. Modern Physics Letters B, 2010, 24, 2295-2301.	1.9	48
68	Effect of long aging on the resistivity properties of optimally doped YBa ₂ Cu ₃ O _{7-δ} single crystals. Solid State Communications, 2013, 170, 6-9.	1.9	48
69	Transport anisotropy and pseudo-gap state in oxygen deficient ReBa ₂ Cu ₃ O _{7-δ} (Re=Y, Ho) single crystals. Journal of Alloys and Compounds, 2008, 464, 58-66.	5.5	47
70	Fluctuation conductivity of oxygen underdoped YBa ₂ Cu ₃ O _{7-δ} single crystals. Physica B: Condensed Matter, 2014, 436, 88-90.	2.7	47
71	Metal-to-insulator transition in Y _{1-x} Pr _x Ba ₂ Cu ₃ O _{7-δ} single crystals with various praseodymium contents. Physica C: Superconductivity and Its Applications, 2013, 485, 89-91.	1.2	46
72	INFLUENCE OF LONGITUDINAL MAGNETIC FIELD ON THE FLUCTUATION CONDUCTIVITY IN SLIGHTLY Al-DOPED YBa ₂ Cu _{3-z} Al _z O _{7-δ} SINGLE CRYSTALS WITH A GIVEN TOPOLOGY OF PLANE DEFECTS. Modern Physics Letters B, 2011, 25, 2131-2136.	1.9	46

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73	Relaxation of the normal electrical resistivity induced by high-pressure in strongly underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ single crystals. <i>Physica B: Condensed Matter</i> , 2012, 407, 4470-4472.	2.7	45
74	Nuclear wastefrom materials: Atomistic simulation case studies. <i>Journal of Nuclear Materials</i> , 2013, 441, 29-39.	2.7	45
75	Experimental synthesis and density functional theory investigation of radiation tolerance of $\text{Zr}_3(\text{Al}_{1-x}\text{S}_x)_2\text{C}_2\text{MAX}$ 3.8 phases. <i>Journal of the American Ceramic Society</i> , 2017, 100, 1377-1387.	3.8	45
76	Excess conductivity and pseudo-gap state in YBCO single crystals slightly doped with Al and Pr. <i>Journal of Materials Science: Materials in Electronics</i> , 2007, 18, 811-815.	2.2	44
77	Defect process and lithium diffusion in Li_2TiO_3 . <i>Solid State Ionics</i> , 2018, 327, 93-98.	2.7	43
78	Evolution of the Fishtail-Effect in Pure and Ag-doped MG-YBCO. <i>Journal of Low Temperature Physics</i> , 2010, 161, 387-394.	1.4	42
79	Effect of small oxygen deficiency on the para-coherent transition and 2D \rightarrow 3D crossover in untwinned $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ single crystals. <i>Journal of Alloys and Compounds</i> , 2011, 509, 4553-4556.	5.5	41
80	A-centers in silicon studied with hybrid density functional theory. <i>Applied Physics Letters</i> , 2013, 103, 052101.	3.3	40
81	Effect of high pressure on the electrical resistivity of optimally doped $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ single crystals with unidirectional planar defects. <i>Physica B: Condensed Matter</i> , 2013, 422, 33-35.	2.7	40
82	Effect of high pressure on the metal-dielectric transition and the pseudo-gap temperature range in oxygen deficient $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ single crystals. <i>Journal of Materials Science: Materials in Electronics</i> , 2011, 22, 20-24.	2.2	39
83	Peculiarities of pseudogap in $\text{Y}_{0.95}\text{Pr}_{0.05}\text{Ba}_2\text{Cu}_3\text{O}_{7-x}$ single crystals under pressure up to 1.7 GPa. <i>Scientific Reports</i> , 2019, 9, 20424.	3.3	39
84	Resistive investigation of pseudogap state in non-stoichiometric $\text{ReBa}_2\text{Cu}_3\text{O}_{7-x}$ ($\text{Re}=\text{Y}, \text{Ho}$) single crystals with account for BCS \rightarrow BEC crossover. <i>Journal of Alloys and Compounds</i> , 2009, 485, L21-L23.	5.5	38
85	Carbon related defects in irradiated silicon revisited. <i>Scientific Reports</i> , 2014, 4, 4909.	3.3	38
86	A high-entropy manganite in an ordered nanocomposite for long-term application in solid oxide cells. <i>Nature Communications</i> , 2021, 12, 2660.	12.8	37
87	Lithium diffusion in Li_5FeO_4 . <i>Scientific Reports</i> , 2018, 8, 5832.	3.3	36
88	Defect chemistry of doped bixbyite oxides. <i>Solid State Sciences</i> , 2007, 9, 588-593.	3.2	35
89	Defect processes in F and Cl doped anatase TiO_2 . <i>Scientific Reports</i> , 2019, 9, 19970.	3.3	35
90	Atomic scale simulations of arsenic \rightarrow vacancy complexes in germanium and silicon. <i>Materials Science in Semiconductor Processing</i> , 2006, 9, 536-540.	4.0	34

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91	Li ₂ SnO ₃ as a Cathode Material for Lithium-ion Batteries: Defects, Lithium Ion Diffusion and Dopants. Scientific Reports, 2018, 8, 12621.	3.3	34
92	Chemically stable new MAX phase V ₂ SnC: a damage and radiation tolerant TBC material. RSC Advances, 2020, 10, 43783-43798.	3.6	34
93	Robust Inorganic Hole Transport Materials for Organic and Perovskite Solar Cells: Insights into Materials Electronic Properties and Device Performance. Solar Rrl, 2021, 5, 2000555.	5.8	34
94	Defects, Dopants and Sodium Mobility in Na ₂ MnSiO ₄ . Scientific Reports, 2018, 8, 14669.	3.3	33
95	Defects and dopant properties of Li ₃ V ₂ (PO ₄) ₃ . Scientific Reports, 2019, 9, 333.	3.3	33
96	Intrinsic defect processes and elastic properties of Ti ₃ AC ₂ (A = Al, Si, Ga, Ge, In, Sn) MAX phases. Journal of Applied Physics, 2018, 123, .	2.5	31
97	A thermodynamic approach of self- and hetero-diffusion in GaAs: connecting point defect parameters with bulk properties. RSC Advances, 2016, 6, 53324-53330.	3.6	30
98	Defects and lithium migration in Li ₂ CuO ₂ . Scientific Reports, 2018, 8, 6754.	3.3	30
99	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.	8.0	30
100	Preparation of hydrogen, fluorine and chlorine doped and co-doped titanium dioxide photocatalysts: a theoretical and experimental approach. Scientific Reports, 2021, 11, 5700.	3.3	30
101	Engineering the free vacancy and active donor concentrations in phosphorus and arsenic double donor-doped germanium. Journal of Applied Physics, 2008, 104, .	2.5	29
102	Impurity diffusion, point defect engineering, and surface/interface passivation in germanium. Annalen Der Physik, 2012, 524, 123-132.	2.4	29
103	Solution combustion synthesis of nano-catalysts with a hierarchical structure. Journal of Catalysis, 2018, 364, 112-124.	6.2	29
104	Engineering Transport in Manganites by Tuning Local Nonstoichiometry in Grain Boundaries. Advanced Materials, 2019, 31, e1805360.	21.0	29
105	Diffusion of tin in germanium: A GGA+ <i>U</i> approach. Applied Physics Letters, 2011, 99, .	3.3	28
106	Point defect engineering strategies to retard phosphorous diffusion in germanium. Physical Chemistry Chemical Physics, 2013, 15, 367-371.	2.8	28
107	Defect Chemistry and Li-ion Diffusion in Li ₂ RuO ₃ . Scientific Reports, 2019, 9, 550.	3.3	28
108	Defects, dopants and Li-ion diffusion in Li ₂ SiO ₃ . Solid State Ionics, 2019, 335, 61-66.	2.7	28

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109	Defects, Lithium Mobility and Tetravalent Dopants in the Li ₃ NbO ₄ Cathode Material. Scientific Reports, 2019, 9, 2192.	3.3	28
110	Connecting point defect parameters with bulk properties to describe diffusion in solids. Applied Physics Reviews, 2016, 3, .	11.3	27
111	Structural and optical properties of the recently synthesized (Zr ₃ ~x Ti x)AlC ₂ MAX phases. Journal of Materials Science: Materials in Electronics, 2017, 28, 3386-3393.	2.2	27
112	A roadmap of strain in doped anatase TiO ₂ . Scientific Reports, 2018, 8, 12790.	3.3	27
113	Effects of Al substitution by Si in Ti ₃ AlC ₂ nanolaminate. Scientific Reports, 2021, 11, 3410.	3.3	27
114	Phase stability and the arsenic vacancy defect in In _x Ga _{1-x} As. Physical Review B, 2011, 84, .	3.2	26
115	Composition and temperature dependence of self-diffusion in Si ₁ ~x Ge x alloys. Scientific Reports, 2017, 7, 1374.	3.3	26
116	Insights into the physical properties of a new 211 MAX phase Nb ₂ CuC. Journal of Physics and Chemistry of Solids, 2021, 149, 109759.	4.0	26
117	Concentration of intrinsic defects and self-diffusion in GaSb. Journal of Applied Physics, 2008, 104, 093714.	2.5	25
118	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.	3.5	25
119	New atomic scale simulation models for hydroxides and oxyhydroxides. Journal of Materials Science, 2006, 41, 675-687.	3.7	24
120	Structure of Sn ₁ ~xGex random alloys as obtained from the coherent potential approximation. Journal of Applied Physics, 2011, 110, 036105.	2.5	24
121	Modelling zirconium hydrides using the special quasirandom structure approach. Physical Chemistry Chemical Physics, 2013, 15, 7599.	2.8	24
122	Hydrogen and nitrogen codoping of anatase TiO ₂ for efficiency enhancement in organic solar cells. Scientific Reports, 2017, 7, 17839.	3.3	24
123	Defects, Dopants and Lithium Mobility in Li ₉ V ₃ (P ₂ O ₇) ₃ (PO ₄) ₂ . Scientific Reports, 2018, 8, 8140.	3.3	23
124	Formation and evolution of oxygen-vacancy clusters in lead and tin doped silicon. Journal of Applied Physics, 2012, 111, .	2.5	22
125	Vacancy-oxygen defects in silicon: the impact of isovalent doping. Journal of Materials Science: Materials in Electronics, 2014, 25, 2395-2410.	2.2	22
126	Diffusion in energy materials: Governing dynamics from atomistic modelling. Applied Physics Reviews, 2017, 4, .	11.3	22

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127	Defect Chemistry and Na-Ion Diffusion in Na ₃ Fe ₂ (PO ₄) ₃ Cathode Material. <i>Materials</i> , 2019, 12, 1348.	2.9	22
128	Li ₃ SbO ₄ lithium-ion battery material: Defects, lithium ion diffusion and tetravalent dopants. <i>Materials Chemistry and Physics</i> , 2019, 225, 34-41.	4.0	22
129	Atomic scale simulations of donor-vacancy pairs in germanium. <i>Journal of Materials Science: Materials in Electronics</i> , 2007, 18, 763-768.	2.2	20
130	Effect of carbon on dopant-vacancy pair stability in germanium. <i>Semiconductor Science and Technology</i> , 2011, 26, 095017.	2.0	20
131	Impact of doping on the ionic conductivity of ceria: A comprehensive model. <i>Journal of Chemical Physics</i> , 2013, 138, 224705.	3.0	20
132	Influence of planar and point defects on the basal-plane conductivity of HoBaCuO single crystals. <i>Physica C: Superconductivity and Its Applications</i> , 2015, 516, 58-61.	1.2	20
133	Modelling solid solutions with cluster expansion, special quasirandom structures, and thermodynamic approaches. <i>Applied Physics Reviews</i> , 2017, 4, 041301.	11.3	20
134	Na ₃ V(PO ₄) ₂ cathode material for Na ion batteries: Defects, dopants and Na diffusion. <i>Solid State Ionics</i> , 2019, 336, 75-79.	2.7	20
135	312 MAX Phases: Elastic Properties and Lithiation. <i>Materials</i> , 2019, 12, 4098.	2.9	20
136	A thermodynamic approach to self-diffusion in silicon: Evidence of a single diffusion mechanism?. <i>Materials Chemistry and Physics</i> , 2016, 181, 204-208.	4.0	19
137	Self-diffusion in garnet-type Li ₇ La ₃ Zr ₂ O ₁₂ solid electrolytes. <i>Scientific Reports</i> , 2021, 11, 451.	3.3	19
138	Unexpected relationship between interlayer distances and surface/cleavage energies in $\hat{3}\langle i \rangle\langle /i \rangle$ TiAl: density functional study. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 265009.	1.8	18
139	Influence of atomic structure on the nano-nickel-based catalyst activity produced by solution combustion synthesis in the hydrogenation of maleic acid. <i>Journal of Catalysis</i> , 2017, 348, 9-21.	6.2	18
140	Special quasirandom structures for gadolinia-doped ceria and related materials. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 11737.	2.8	17
141	Fluctuation conductivity and possible pseudogap state in FeAs-based superconductor EuFeAsO _{0.85} F _{0.15} . <i>Materials Research Express</i> , 2016, 3, 076001.	1.6	17
142	Optimized hydrogen positions for aluminium and iron containing hydroxide minerals. <i>Journal of Materials Science</i> , 2007, 42, 2024-2029.	3.7	16
143	Extrinsic doping in silicon revisited. <i>Applied Physics Letters</i> , 2010, 96, 242107.	3.3	16
144	Doping strategies to control A-centres in silicon: insights from hybrid density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 8487.	2.8	16

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145	Anomaly detection in time series data using a combination of wavelets, neural networks and Hilbert transform. , 2015, , .		16
146	Describing oxygen self-diffusion in PuO ₂ by connecting point defect parameters with bulk properties. Journal of Materials Science: Materials in Electronics, 2015, 26, 3287-3290.	2.2	16
147	Modification of superconducting and resistive properties of HoBa ₂ Cu ₃ O _{7-x} single crystals under application-removal of high hydrostatic pressure. Modern Physics Letters B, 2016, 30, 1650188.	1.9	16
148	Different diffusion mechanisms of oxygen in ReBa ₂ Cu ₃ O _{7-x} (Re = Y, Ho) single crystals. Physica C: Superconductivity and Its Applications, 2017, 536, 26-29.	1.2	16
149	Diffusion and Dopant Activation in Germanium: Insights from Recent Experimental and Theoretical Results. Applied Sciences (Switzerland), 2019, 9, 2454.	2.5	16
150	Impact of boron and indium doping on the structural, electronic and optical properties of SnO ₂ . Scientific Reports, 2021, 11, 13031.	3.3	16
151	Special quasirandom structures for binary/ternary group IV random alloys. Chemical Physics Letters, 2010, 493, 97-102.	2.6	15
152	Carbon, oxygen and intrinsic defect interactions in germanium-doped silicon. Semiconductor Science and Technology, 2011, 26, 105024.	2.0	15
153	Doping and cluster formation in diamond. Journal of Applied Physics, 2011, 110, .	2.5	15
154	Defect engineering of the oxygen-vacancy clusters formation in electron irradiated silicon by isovalent doping: An infrared perspective. Journal of Applied Physics, 2012, 112, .	2.5	15
155	Defect configurations of high-k cations in germanium. Journal of Applied Physics, 2012, 111, 023714.	2.5	15
156	Co-doping with antimony to control phosphorous diffusion in germanium. Journal of Applied Physics, 2013, 113, .	2.5	15
157	G-centers in irradiated silicon revisited: A screened hybrid density functional theory approach. Journal of Applied Physics, 2014, 115, .	2.5	15
158	Connecting bulk properties of germanium with the behavior of self- and dopant diffusion. Materials Science in Semiconductor Processing, 2015, 36, 179-183.	4.0	15
159	Toward Defect Engineering Strategies to Optimize Energy and Electronic Materials. Applied Sciences (Switzerland), 2017, 7, 674.	2.5	15
160	<i>Ab initio</i> modeling of MAX phase solid solutions using the special quasirandom structure approach. Physical Chemistry Chemical Physics, 2018, 20, 1173-1180.	2.8	15
161	Defect, Diffusion and Dopant Properties of NaNiO ₂ : Atomistic Simulation Study. Energies, 2019, 12, 3094.	3.1	15
162	Vacancy-indium clusters in implanted germanium. Chemical Physics Letters, 2010, 490, 38-40.	2.6	14

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163	Ultrafast palladium diffusion in germanium. <i>Journal of Materials Chemistry A</i> , 2015, 3, 3832-3838.	10.3	14
164	Modeling indium diffusion in germanium by connecting point defect parameters with bulk properties. <i>Journal of Materials Science: Materials in Electronics</i> , 2015, 26, 2113-2116.	2.2	14
165	Thermodynamic calculations of oxygen self-diffusion in mixed-oxide nuclear fuels. <i>RSC Advances</i> , 2016, 6, 74018-74027.	3.6	14
166	The encapsulation selectivity for anionic fission products imparted by an electride. <i>Scientific Reports</i> , 2019, 9, 13612.	3.3	14
167	Behavior of Li-ion on the surface of Ti_3C_2 (T = O, S, Se, F, Cl, Br) MXene: Diffusion barrier and conductive pathways. <i>Journal of Applied Physics</i> , 2021, 130, .	2.5	14
168	LOCALIZATION EFFECT AND PSEUDOGAP IN PRASEODYMIUM DOPED $Y_{1-z}Pr_zBa_2CuO_3$ SINGLE CRYSTALS. <i>Modern Physics Letters B</i> , 2012, 26, 1250163.		
169	Electronegativity and doping in $Si_{1-x}Ge_x$ alloys. <i>Scientific Reports</i> , 2020, 10, 7459.	3.3	13
170	Optical response, lithiation and charge transfer in Sn-based 211 MAX phases with electron localization function. <i>Journal of Materials Research and Technology</i> , 2022, 18, 2470-2479.	5.8	13
171	Defect engineering strategies for germanium. <i>Journal of Materials Science: Materials in Electronics</i> , 2013, 24, 1741-1747.	2.2	12
172	Antisites in III-V semiconductors: Density functional theory calculations. <i>Journal of Applied Physics</i> , 2014, 116, .	2.5	12
173	Stress-enhanced lithiation in MAX compounds for battery applications. <i>Applied Materials Today</i> , 2017, 9, 192-195.	4.3	12
174	Defects, Diffusion, and Dopants in $Li_2Ti_6O_{13}$: Atomistic Simulation Study. <i>Materials</i> , 2019, 12, 2851.	2.9	12
175	Defect Process, Dopant Behaviour and Li Ion Mobility in the Li_2MnO_3 Cathode Material. <i>Energies</i> , 2019, 12, 1329.	3.1	12
176	Ru-Doped Single Walled Carbon Nanotubes as Sensors for SO_2 and H_2S Detection. <i>Chemosensors</i> , 2021, 9, 120.	3.6	12
177	Interaction of oxygen vacancies in yttrium germanates. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14630.	2.8	11
178	Impact of isovalent defect engineering strategies on carbon-related clusters in silicon. <i>Journal of Materials Science: Materials in Electronics</i> , 2013, 24, 1696-1701.	2.2	11
179	Phosphorous "vacancy" oxygen defects in silicon. <i>Journal of Materials Chemistry A</i> , 2013, 1, 11384.	10.3	11
180	Antisites and anisotropic diffusion in GaAs and GaSb. <i>Applied Physics Letters</i> , 2013, 103, 142107.	3.3	11

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181	Impact of isovalent doping on radiation defects in silicon. Journal of Applied Physics, 2013, 114, .	2.5	11
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