Navaratnarajah Kuganathan

List of Publications by Year
in descending order

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106 papers	2,706 citations	304368 22 h-index	189595 50 g-index
107 all docs	107 docs citations	107 times ranked	3186 citing authors

#	Article	IF	Citations
1	Ultrafast epitaxial growth of CuO nanowires using atmospheric pressure plasma with enhanced electrocatalytic and photocatalytic activities. Nano Select, 2022, 3, 627-642.	1.9	3
2	Defects, dopants and lithium incorporation in LiPON electrolyte. Computational Materials Science, 2022, 202, 111000.	1.4	5
3	Theoretical investigation of nitrogen-vacancy defects in silicon. AIP Advances, 2022, 12, .	0.6	4
4	Intrinsic Defects, Diffusion and Dopants in AVSi2O6 (A = Li and Na) Electrode Materials. Batteries, 2022, 8, 20.	2.1	1
5	Activation of CO2 on the Surfaces of Bare, Ti-Adsorbed and Ti-Doped C60. Fuels, 2022, 3, 176-183.	1.3	1
6	Computational Study of Crystallography, Defects, Ion Migration and Dopants in Almandine Garnet. Physchem, 2022, 2, 43-51.	0.5	1
7	Chalcogen Atom-Doped Graphene and Its Performance in N2 Activation. Surfaces, 2022, 5, 228-237.	1.0	0
8	Nitrogen-vacancy defects in germanium. AIP Advances, 2022, 12, 045110.	0.6	2
9	Formation, doping, and lithium incorporation in LiFePO4. AIP Advances, 2022, 12, .	0.6	4
10	Defect Properties of Li2NiGe3O8. Clean Technologies, 2022, 4, 619-628.	1.9	1
11	Adsorption of lead on the surfaces of pristine and B, Si and N-doped graphene. Physica B: Condensed Matter, 2021, 600, 412639.	1.3	21
12	Atomistic modeling approach to the thermodynamics of sodium silicate glasses. Journal of the American Ceramic Society, 2021, 104, 1331-1344.	1.9	3
13	Removal of Lead by Oxidized Graphite. Journal of Carbon Research, 2021, 7, 23.	1.4	4
14	Defect energetics in the SrTiO3-LaCrO3 system. Solid State Ionics, 2021, 361, 115570.	1.3	9
15	Defects, diffusion and dopants in the ceramic mineral â€œLime- Feldsparâ€• Journal of Asian Ceramic Societies, 2021, 9, 570-577.	1.0	3
16	Defects, diffusion, dopants and encapsulation of Na in NaZr2(PO4)3. Materialia, 2021, 16, 101039.	1.3	5
17	Defect and dopant properties in CaMnO3. AIP Advances, 2021, 11, 055106.	0.6	5
18	Ru-Doped Single Walled Carbon Nanotubes as Sensors for SO2 and H2S Detection. Chemosensors, 2021, 9, 120.	1.8	12

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19	Substitutional carbon-dioxygen center in irradiated silicon. Materials Science in Semiconductor Processing, 2021, 127, 105661.	1.9	1
20	One-dimensional polyhedral chain of ThCl6 encapsulated within single-walled carbon nanotubes. AIP Advances, 2021, 11, 065117.	0.6	1
21	One-dimensional yttrium silicide electride (Y5Si3:eâ^') for encapsulation of volatile fission products. Journal of Applied Physics, 2021, 129, .	1.1	2
22	Impact of oxygen on gallium doped germanium. AIP Advances, 2021, 11, 065122.	0.6	3
23	Defect Properties and Lithium Incorporation in Li2ZrO3. Energies, 2021, 14, 3963.	1.6	6
24	Interstitial lithium doping in SrTiO₃. AIP Advances, 2021, 11, 075029.	0.6	2
25	Defects, diffusion and dopants in Li8SnO6. Heliyon, 2021, 7, e07460.	1.4	3
26	Simulation-Based Defect Engineering in â€œÎ±-Spodumeneâ€• ChemEngineering, 2021, 5, 57.	1.0	0
27	Encapsulation and Adsorption of Halogens into Single-Walled Carbon Nanotubes. Micro, 2021, 1, 140-150.	0.9	2
28	Oxygen migration in doped BaGdInO4. Solid State Ionics, 2021, 369, 115729.	1.3	0
29	Self-diffusion in garnet-type Li7La3Zr2O12 solid electrolytes. Scientific Reports, 2021, 11, 451.	1.6	19
30	Formation of atomic fluorine anions in 12CaOÂ·7Al2O3. AIP Advances, 2021, 11, 015146.	0.6	0
31	Graphene Synthesis and Its Recent Advances in Applicationsâ€”A Review. Journal of Carbon Research, 2021, 7, 76.	1.4	17
32	Mayenite Electrides and Their Doped Forms for Oxygen Reduction Reaction in Solid Oxide Fuel Cells. Energies, 2020, 13, 4978.	1.6	0
33	Atomic-scale studies of garnet-type Mg3Fe2Si3O12: Defect chemistry, diffusion and dopant properties. Journal of Power Sources Advances, 2020, 3, 100016.	2.6	2
34	Defects, Diffusion and Dopants in Sillimanite. Minerals (Basel, Switzerland), 2020, 10, 857.	0.8	1
35	Defects and Calcium Diffusion in Wollastonite. Chemistry, 2020, 2, 937-946.	0.9	0
36	Defect, transport, and dopant properties of andradite garnet Ca3Fe2Si3O12. AIP Advances, 2020, 10, .	0.6	6

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37	Encapsulation of volatile fission products in a two-dimensional dicalcium nitride electride. Journal of Applied Physics, 2020, 128, 045112.	1.1	3
38	Tuning the electronic properties of C12A7 via Sn doping and encapsulation. Journal of Materials Science: Materials in Electronics, 2020, 31, 21203-21213.	1.1	1
39	Hydrogen Adsorption on Ru-Encapsulated, -Doped and -Supported Surfaces of C60. Surfaces, 2020, 3, 408-422.	1.0	5
40	The Interstitial Carbonâ€“Dioxygen Center in Irradiated Silicon. Crystals, 2020, 10, 1005.	1.0	3
41	Electronegativity and doping in Si1-xGex alloys. Scientific Reports, 2020, 10, 7459.	1.6	13
42	Defects and Dopants in CaFeSi2O6: Classical and DFT Simulations. Energies, 2020, 13, 1285.	1.6	11
43	Structural, defect, transport and dopant properties of AgNbO 3. ChemNanoMat, 2020, 6, 1337-1345.	1.5	7
44	Encapsulation and substitution of Fe in C12A7 (12CaOâ‹…7Al2O3). AIP Advances, 2020, 10, 015242.	0.6	3
45	Computer modeling investigation of MgV2O4 for Mg-ion batteries. Journal of Applied Physics, 2020, 127, 035106.	1.1	10
46	Lithium Storage in Nanoporous Complex Oxide 12CaOâ€¢7Al2O3 (C12A7). Energies, 2020, 13, 1547.	1.6	4
47	Impact of local composition on the energetics of E-centres in Si1â^'xGex alloys. Scientific Reports, 2019, 9, 10849.	1.6	4
48	Atomistic Simulations of the Defect Chemistry and Self-Diffusion of Li-ion in LiAlO2. Energies, 2019, 12, 2895.	1.6	8
49	Defect Chemistry, Sodium Diffusion and Doping Behaviour in NaFeO2 Polymorphs as Cathode Materials for Na-Ion Batteries: A Computational Study. Materials, 2019, 12, 3243.	1.3	11
50	Theoretical Modeling of Defects, Dopants, and Diffusion in the Mineral Ilmenite. Minerals (Basel,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 2	0.8	5
51	The encapsulation selectivity for anionic fission products imparted by an electride. Scientific Reports, 2019, 9, 13612.	1.6	14
52	Mg6MnO8 as a Magnesium-Ion Battery Material: Defects, Dopants and Mg-Ion Transport. Energies, 2019, 12, 3213.	1.6	10
53	A Computational Study of Defects, Li-Ion Migration and Dopants in Li2ZnSiO4 Polymorphs. Crystals, 2019, 9, 563.	1.0	5
54	Stability of Coinage Metals Interacting with C60. Nanomaterials, 2019, 9, 1484.	1.9	4

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55	Defects, Diffusion, and Dopants in Li2Ti6O13: Atomistic Simulation Study. Materials, 2019, 12, 2851.	1.3	12
56	Defect, Diffusion and Dopant Properties of NaNiO2: Atomistic Simulation Study. Energies, 2019, 12, 3094.	1.6	15
57	Encapsulation of cadmium telluride nanocrystals within single walled carbon nanotubes. Inorganica Chimica Acta, 2019, 488, 246-254.	1.2	8
58	Defect Chemistry and Li-ion Diffusion in Li2RuO3. Scientific Reports, 2019, 9, 550.	1.6	28
59	Diffusion and Dopant Activation in Germanium: Insights from Recent Experimental and Theoretical Results. Applied Sciences (Switzerland), 2019, 9, 2454.	1.3	16
60	Defect Chemistry and Na-Ion Diffusion in Na3Fe2(PO4)3 Cathode Material. Materials, 2019, 12, 1348.	1.3	22
61	Dinitrogen activation by zirconium dimer loaded C60. AIP Advances, 2019, 9, 055331.	0.6	0
62	Technetium Encapsulation by A Nanoporous Complex Oxide 12CaOâ€¢7Al2O3 (C12A7). Nanomaterials, 2019, 9, 816.	1.9	11
63	Defect Process, Dopant Behaviour and Li Ion Mobility in the Li2MnO3 Cathode Material. Energies, 2019, 12, 1329.	1.6	12
64	Thermal and diffusional properties of (Th,Np)O2 and (U,Np)O2 mixed oxides. Journal of Nuclear Materials, 2019, 521, 89-98.	1.3	6
65	Encapsulation of heavy metals by a nanoporous complex oxide 12CaOâ€‰Â·â€‰7Al2O3. Journal of Applied Physics, 2019, 125, .	1.1	7
66	Defects, dopants and Mg diffusion in MgTiO3. Scientific Reports, 2019, 9, 4394.	1.6	63
67	Defects, dopants and Li-ion diffusion in Li2SiO3. Solid State Ionics, 2019, 335, 61-66.	1.3	28
68	Na3V(PO4)2 cathode material for Na ion batteries: Defects, dopants and Na diffusion. Solid State Ionics, 2019, 336, 75-79.	1.3	20
69	Defects, Lithium Mobility and Tetravalent Dopants in the Li3NbO4 Cathode Material. Scientific Reports, 2019, 9, 2192.	1.6	28
70	Cadmium trapping by C60 and B-, Si-, and N-doped C60. Journal of Applied Physics, 2019, 125, 054302.	1.1	7
71	Li3SbO4 lithium-ion battery material: Defects, lithium ion diffusion and tetravalent dopants. Materials Chemistry and Physics, 2019, 225, 34-41.	2.0	22
72	Defects and dopant properties of Li3V2(PO4)3. Scientific Reports, 2019, 9, 333.	1.6	33

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73	Encapsulation of Cadmium Selenide Nanocrystals in Biocompatible Nanotubes: DFT Calculations, Xâ€ray Diffraction Investigations, and Confocal Fluorescence Imaging. ChemistryOpen, 2018, 7, 144-158.	0.9	15
74	Lithium diffusion in Li5FeO4. Scientific Reports, 2018, 8, 5832.	1.6	36
75	Trapping of volatile fission products by C60. Carbon, 2018, 132, 477-485.	5.4	16
76	Defect process and lithium diffusion in Li2TiO3. Solid State Ionics, 2018, 327, 93-98.	1.3	43
77	Defects, Dopants and Sodium Mobility in Na2MnSiO4. Scientific Reports, 2018, 8, 14669.	1.6	33
78	Defects, Dopants and Lithium Mobility in Li 9 V 3 (P 2 O 7) 3 (PO 4) 2. Scientific Reports, 2018, 8, 8140.	1.6	23
79	Phase stability, electronic structures and elastic properties of (U,Np)O2 and (Th,Np)O2 mixed oxides. Physical Chemistry Chemical Physics, 2018, 20, 18707-18717.	1.3	9
80	Helium trapping and clustering in ThO2. Journal of Nuclear Materials, 2018, 507, 288-296.	1.3	6
81	Defects and lithium migration in Li2CuO2. Scientific Reports, 2018, 8, 6754.	1.6	30
82	Li2SnO3 as a Cathode Material for Lithium-ion Batteries: Defects, Lithium Ion Diffusion and Dopants. Scientific Reports, 2018, 8, 12621.	1.6	34
83	Fission gas in thoria. Journal of Nuclear Materials, 2017, 485, 47-55.	1.3	13
84	Fluorescenceâ€Lifetime Imaging and Superâ€Resolution Microscopies Shed Light on the Directedâ€and Selfâ€Assembly of Functional Porphyrins onto Carbon Nanotubes and Flat Surfaces. Chemistry - A European Journal, 2017, 23, 9772-9789.	1.7	16
85	Energetics of halogen impurities in thorium dioxide. Journal of Nuclear Materials, 2017, 495, 192-201.	1.3	5
86	A computational study on the superionic behaviour of ThO₂. Physical Chemistry Chemical Physics, 2016, 18, 31494-31504.	1.3	17
87	Electride support boosts nitrogen dissociation over ruthenium catalyst and shifts the bottleneck in ammonia synthesis. Nature Communications, 2015, 6, 6731.	5.8	529
88	Enhanced N₂ Dissociation on Ru-Loaded Inorganic Electride. Journal of the American Chemical Society, 2014, 136, 2216-2219.	6.6	52
89	Activation and splitting of carbon dioxide on the surface of an inorganic electride material. Nature Communications, 2013, 4, 2378.	5.8	151
90	Defect chemistry and lithium-ion migration in polymorphs of the cathode material Li2MnSiO4. Journal of Materials Chemistry A, 2013, 1, 4207.	5.2	113

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91	Exploring Pathways for Activation of Carbon Monoxide by Palladium Iminophosphines. ChemPlusChem, 2013, 78, 1413-1420.	1.3	0
92	Interactions and Reactions of Transition Metal Clusters with the Interior of Single-Walled Carbon Nanotubes Imaged at the Atomic Scale. Journal of the American Chemical Society, 2012, 134, 3073-3079.	6.6	83
93	Aberration corrected imaging of a carbon nanotube encapsulated Lindqvist Ion and correlation with Density Functional Theory. Journal of Physics: Conference Series, 2012, 371, 012018.	0.3	1
94	High-precision imaging of an encapsulated Lindqvist ion and correlation of its structure and symmetry with quantum chemical calculations. Nanoscale, 2012, 4, 1190.	2.8	11
95	Interactions Between Amino Acidâ€Tagged Naphthalenediimide and Single Walled Carbon Nanotubes for the Design and Construction of New Bioimaging Probes. Advanced Functional Materials, 2012, 22, 503-518.	7.8	49
96	Structure and Lithium Transport Pathways in Li₂FeSiO₄ Cathodes for Lithium Batteries. Journal of the American Chemical Society, 2011, 133, 13031-13035.	6.6	277
97	Chemical Analysis ofDatura MetelLeaves and Investigation of the Acute Toxicity on Grasshoppers and Red Ants. E-Journal of Chemistry, 2011, 8, 107-112.	0.4	14
98	Self-assembly of a sulphur-terminated graphene nanoribbon within a single-walled carbon nanotube. Nature Materials, 2011, 10, 687-692.	13.3	253
99	DFT Modelling of Tripeptides (Lysine-Tryptophan-Lysine) Interacting with Single Walled Carbon Nanotubes. E-Journal of Chemistry, 2010, 7, 870-874.	0.4	1
100	Antimony Selenide Crystals Encapsulated within Single Walled Carbon Nanotubes-A DFT Study. E-Journal of Chemistry, 2009, 6, S147-S152.	0.4	6
101	1D lead iodide crystals encapsulated within single walled carbon nanotubes. International Journal of Quantum Chemistry, 2009, 109, 171-175.	1.0	4
102	Li₂MnSiO₄ Lithium Battery Material: Atomic-Scale Study of Defects, Lithium Mobility, and Trivalent Dopants. Chemistry of Materials, 2009, 21, 5196-5202.	3.2	160
103	Mercury telluride crystals encapsulated within single walled carbon nanotubes: A density functional study. International Journal of Quantum Chemistry, 2008, 108, 797-807.	1.0	13
104	Interactions between tripodal porphyrin hosts and single walled carbon nanotubes: an experimental and theoretical (DFT) account. Journal of Materials Chemistry, 2008, 18, 2781.	6.7	17
105	Crystal structure of low-dimensional Cu(i) iodide: DFT prediction of cuprophilic interactions. Chemical Communications, 2008, , 2432.	2.2	31
106	Dinitrogen fixation and activation by Ti and Zr atoms, clusters and complexes. New Journal of Chemistry, 2006, 30, 1253.	1.4	36