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	Electride support boosts nitrogen dissociation over ruthenium catalyst and shifts the bottleneck in ammonia synthesis. Nature Communications, 2015, 6, 6731.	5.8	529
2	Structure and Lithium Transport Pathways in Li₂FeSiO₄ Cathodes for Lithium Batteries. Journal of the American Chemical Society, 2011, 133, 13031-13035.	6.6	277
3	Self-assembly of a sulphur-terminated graphene nanoribbon within a single-walled carbon nanotube. Nature Materials, 2011, 10, 687-692.	13.3	253
4	Li₂MnSiO₄ Lithium Battery Material: Atomic-Scale Study of Defects, Lithium Mobility, and Trivalent Dopants. Chemistry of Materials, 2009, 21, 5196-5202.	3.2	160
5	Activation and splitting of carbon dioxide on the surface of an inorganic electride material. Nature Communications, 2013, 4, 2378.	5.8	151
6	Defect chemistry and lithium-ion migration in polymorphs of the cathode material Li2MnSiO4. Journal of Materials Chemistry A, 2013, 1, 4207.	5.2	113
7	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
8	Defects, dopants and Mg diffusion in MgTiO3. Scientific Reports, 2019, 9, 4394.	1.6	63
9	Enhanced N₂ Dissociation on Ru-Loaded Inorganic Electride. Journal of the American Chemical Society, 2014, 136, 2216-2219.	6.6	52
10	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
11	Defect process and lithium diffusion in Li2TiO3. Solid State Ionics, 2018, 327, 93-98.	1.3	43
12	Dinitrogen fixation and activation by Ti and Zr atoms, clusters and complexes. New Journal of Chemistry, 2006, 30, 1253.	1.4	36
13	Lithium diffusion in Li5FeO4. Scientific Reports, 2018, 8, 5832.	1.6	36
14	Li2SnO3 as a Cathode Material for Lithium-ion Batteries: Defects, Lithium Ion Diffusion and Dopants. Scientific Reports, 2018, 8, 12621.	1.6	34
15	Defects, Dopants and Sodium Mobility in Na2MnSiO4. Scientific Reports, 2018, 8, 14669.	1.6	33
16	Defects and dopant properties of Li3V2(PO4)3. Scientific Reports, 2019, 9, 333.	1.6	33
17	Crystal structure of low-dimensional Cu(i) iodide: DFT prediction of cuprophilic interactions. Chemical Communications, 2008, , 2432.	2.2	31
18	Defects and lithium migration in Li2CuO2. Scientific Reports, 2018, 8, 6754.	1.6	30

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19	Defect Chemistry and Li-ion Diffusion in Li2RuO3. Scientific Reports, 2019, 9, 550.	1.6	28
20	Defects, dopants and Li-ion diffusion in Li2SiO3. Solid State Ionics, 2019, 335, 61-66.	1.3	28
21	Defects, Lithium Mobility and Tetravalent Dopants in the Li3NbO4 Cathode Material. Scientific Reports, 2019, 9, 2192.	1.6	28
22	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
23	Defect Chemistry and Na-Ion Diffusion in Na3Fe2(PO4)3 Cathode Material. Materials, 2019, 12, 1348.	1.3	22
24	Li3SbO4 lithium-ion battery material: Defects, lithium ion diffusion and tetravalent dopants. Materials Chemistry and Physics, 2019, 225, 34-41.	2.0	22
25	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
26	Na3V(PO4)2 cathode material for Na ion batteries: Defects, dopants and Na diffusion. Solid State Ionics, 2019, 336, 75-79.	1.3	20
27	Self-diffusion in garnet-type Li7La3Zr2O12 solid electrolytes. Scientific Reports, 2021, 11, 451.	1.6	19
28	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
29	A computational study on the superionic behaviour of ThO₂. Physical Chemistry Chemical Physics, 2016, 18, 31494-31504.	1.3	17
30	Graphene Synthesis and Its Recent Advances in Applicationsâ€"A Review. Journal of Carbon Research, 2021, 7, 76.	1.4	17
31	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
32	Trapping of volatile fission products by C60. Carbon, 2018, 132, 477-485.	5.4	16
33	Diffusion and Dopant Activation in Germanium: Insights from Recent Experimental and Theoretical Results. Applied Sciences (Switzerland), 2019, 9, 2454.	1.3	16
34	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
35	Defect, Diffusion and Dopant Properties of NaNiO2: Atomistic Simulation Study. Energies, 2019, 12, 3094.	1.6	15
36	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

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37	The encapsulation selectivity for anionic fission products imparted by an electride. Scientific Reports, 2019, 9, 13612.	1.6	14
38	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
39	Fission gas in thoria. Journal of Nuclear Materials, 2017, 485, 47-55.	1.3	13
40	Electronegativity and doping in Si1-xGex alloys. Scientific Reports, 2020, 10, 7459.	1.6	13
41	Defects, Diffusion, and Dopants in Li2Ti6O13: Atomistic Simulation Study. Materials, 2019, 12, 2851.	1.3	12
42	Defect Process, Dopant Behaviour and Li Ion Mobility in the Li2MnO3 Cathode Material. Energies, 2019, 12, 1329.	1.6	12
43	Ru-Doped Single Walled Carbon Nanotubes as Sensors for SO2 and H2S Detection. Chemosensors, 2021, 9, 120.	1.8	12
44	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
45	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
46	Technetium Encapsulation by A Nanoporous Complex Oxide 12CaOâ€¢7Al2O3 (C12A7). Nanomaterials, 2019, 9, 816.	1.9	11
47	Defects and Dopants in CaFeSi2O6: Classical and DFT Simulations. Energies, 2020, 13, 1285.	1.6	11
48	Mg6MnO8 as a Magnesium-Ion Battery Material: Defects, Dopants and Mg-Ion Transport. Energies, 2019, 12, 3213.	1.6	10
49	Computer modeling investigation of MgV2O4 for Mg-ion batteries. Journal of Applied Physics, 2020, 127, 035106.	1.1	10
50	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
51	Defect energetics in the SrTiO3-LaCrO3 system. Solid State Ionics, 2021, 361, 115570.	1.3	9
52	Atomistic Simulations of the Defect Chemistry and Self-Diffusion of Li-ion in LiAlO2. Energies, 2019, 12, 2895.	1.6	8
53	Encapsulation of cadmium telluride nanocrystals within single walled carbon nanotubes. Inorganica Chimica Acta, 2019, 488, 246-254.	1.2	8
54	Encapsulation of heavy metals by a nanoporous complex oxide 12CaOâ€‰Â·â€‰7Al2O3. Journal of Applied Physics, 2019, 125, .	1.1	7

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55	Cadmium trapping by C60 and B-, Si-, and N-doped C60. Journal of Applied Physics, 2019, 125, 054302.	1.1	7
56	Structural, defect, transport and dopant properties of AgNbO 3. ChemNanoMat, 2020, 6, 1337-1345.	1.5	7
57	Antimony Selenide Crystals Encapsulated within Single Walled Carbon Nanotubes-A DFT Study. E-Journal of Chemistry, 2009, 6, S147-S152.	0.4	6
58	Helium trapping and clustering in ThO2. Journal of Nuclear Materials, 2018, 507, 288-296.	1.3	6
59	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
60	Defect, transport, and dopant properties of andradite garnet Ca3Fe2Si3O12. AIP Advances, 2020, 10, .	0.6	6
61	Defect Properties and Lithium Incorporation in Li2ZrO3. Energies, 2021, 14, 3963.	1.6	6
62	Energetics of halogen impurities in thorium dioxide. Journal of Nuclear Materials, 2017, 495, 192-201.	1.3	5
63	Theoretical Modeling of Defects, Dopants, and Diffusion in the Mineral Ilmenite. Minerals (Basel,) Tj ETQq1 1 0.784314 rgBT /Overloc	0.8	5
64	A Computational Study of Defects, Li-Ion Migration and Dopants in Li2ZnSiO4 Polymorphs. Crystals, 2019, 9, 563.	1.0	5
65	Hydrogen Adsorption on Ru-Encapsulated, -Doped and -Supported Surfaces of C60. Surfaces, 2020, 3, 408-422.	1.0	5
66	Defects, diffusion, dopants and encapsulation of Na in NaZr2(PO4)3. Materialia, 2021, 16, 101039.	1.3	5
67	Defect and dopant properties in CaMnO3. AIP Advances, 2021, 11, 055106.	0.6	5
68	Defects, dopants and lithium incorporation in LiPON electrolyte. Computational Materials Science, 2022, 202, 111000.	1.4	5
69	1D lead iodide crystals encapsulated within single walled carbon nanotubes. International Journal of Quantum Chemistry, 2009, 109, 171-175.	1.0	4
70	Impact of local composition on the energetics of E-centres in Si1â^'xGex alloys. Scientific Reports, 2019, 9, 10849.	1.6	4
71	Stability of Coinage Metals Interacting with C60. Nanomaterials, 2019, 9, 1484.	1.9	4
72	Lithium Storage in Nanoporous Complex Oxide 12CaOâ€¢7Al2O3 (C12A7). Energies, 2020, 13, 1547.	1.6	4

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73	Removal of Lead by Oxidized Graphite. Journal of Carbon Research, 2021, 7, 23.	1.4	4
74	Theoretical investigation of nitrogen-vacancy defects in silicon. AIP Advances, 2022, 12, .	0.6	4
75	Formation, doping, and lithium incorporation in LiFePO4. AIP Advances, 2022, 12, .	0.6	4
76	Encapsulation of volatile fission products in a two-dimensional dicalcium nitride electride. Journal of Applied Physics, 2020, 128, 045112.	1.1	3
77	The Interstitial Carbonâ€“Dioxygen Center in Irradiated Silicon. Crystals, 2020, 10, 1005.	1.0	3
78	Encapsulation and substitution of Fe in C12A7 (12CaOâ‹…7Al2O3). AIP Advances, 2020, 10, 015242.	0.6	3
79	Atomistic modeling approach to the thermodynamics of sodium silicate glasses. Journal of the American Ceramic Society, 2021, 104, 1331-1344.	1.9	3
80	Defects, diffusion and dopants in the ceramic mineral â€œLime- Feldsparâ€• Journal of Asian Ceramic Societies, 2021, 9, 570-577.	1.0	3
81	Impact of oxygen on gallium doped germanium. AIP Advances, 2021, 11, 065122.	0.6	3
82	Defects, diffusion and dopants in Li8SnO6. Heliyon, 2021, 7, e07460.	1.4	3
83	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
84	Atomic-scale studies of garnet-type Mg3Fe2Si3O12: Defect chemistry, diffusion and dopant properties. Journal of Power Sources Advances, 2020, 3, 100016.	2.6	2
85	One-dimensional yttrium silicide electride (Y5Si3:eâ¯) for encapsulation of volatile fission products. Journal of Applied Physics, 2021, 129, .	1.1	2
86	Interstitial lithium doping in SrTiO₃. AIP Advances, 2021, 11, 075029.	0.6	2
87	Encapsulation and Adsorption of Halogens into Single-Walled Carbon Nanotubes. Micro, 2021, 1, 140-150.	0.9	2
88	Nitrogen-vacancy defects in germanium. AIP Advances, 2022, 12, 045110.	0.6	2
89	DFT Modelling of Tripeptides (Lysine-Tryptophan-Lysine) Interacting with Single Walled Carbon Nanotubes. E-Journal of Chemistry, 2010, 7, 870-874.	0.4	1
90	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

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91	Defects, Diffusion and Dopants in Sillimanite. Minerals (Basel, Switzerland), 2020, 10, 857.	0.8	1
92	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
93	Substitutional carbon-dioxygen center in irradiated silicon. Materials Science in Semiconductor Processing, 2021, 127, 105661.	1.9	1
94	One-dimensional polyhedral chain of ThCl6 encapsulated within single-walled carbon nanotubes. AIP Advances, 2021, 11, 065117.	0.6	1
95	Intrinsic Defects, Diffusion and Dopants in AVSi2O6 (A = Li and Na) Electrode Materials. Batteries, 2022, 8, 20.	2.1	1
96	Activation of CO2 on the Surfaces of Bare, Ti-Adsorbed and Ti-Doped C60. Fuels, 2022, 3, 176-183.	1.3	1
97	Computational Study of Crystallography, Defects, Ion Migration and Dopants in Almandine Garnet. Physchem, 2022, 2, 43-51.	0.5	1
98	Defect Properties of Li2NiGe3O8. Clean Technologies, 2022, 4, 619-628.	1.9	1
99	Exploring Pathways for Activation of Carbon Monoxide by Palladium Iminophosphines. ChemPlusChem, 2013, 78, 1413-1420.	1.3	0
100	Dinitrogen activation by zirconium dimer loaded C60. AIP Advances, 2019, 9, 055331.	0.6	0
101	Mayenite Electrides and Their Doped Forms for Oxygen Reduction Reaction in Solid Oxide Fuel Cells. Energies, 2020, 13, 4978.	1.6	0
102	Defects and Calcium Diffusion in Wollastonite. Chemistry, 2020, 2, 937-946.	0.9	0
103	Simulation-Based Defect Engineering in â€œÎ±-Spodumeneâ€• ChemEngineering, 2021, 5, 57.	1.0	0
104	Oxygen migration in doped BaGdInO4. Solid State Ionics, 2021, 369, 115729.	1.3	0
105	Formation of atomic fluorine anions in 12CaOÂ·7Al2O3. AIP Advances, 2021, 11, 015146.	0.6	0
106	Chalcogen Atom-Doped Graphene and Its Performance in N2 Activation. Surfaces, 2022, 5, 228-237.	1.0	0