

Ram Devanathan

List of Publications by Year in descending order

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131
papers

5,254
citations

101384

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137
all docs

137
docs citations

137
times ranked

4440
citing authors

#	ARTICLE	IF	CITATIONS
1	Grain-size effects on the deformation in nanocrystalline multi-principal element alloy. <i>Materials Chemistry and Physics</i> , 2022, 277, 125546.	2.0	14
2	Machine-learning-guided descriptor selection for predicting corrosion resistance in multi-principal element alloys. <i>Npj Materials Degradation</i> , 2022, 6, .	2.6	29
3	Uncertainty quantification for Bayesian active learning in rupture life prediction of ferritic steels. <i>Scientific Reports</i> , 2022, 12, 2083.	1.6	5
4	Computational Design of Alloys for Energy Technologies. <i>Jom</i> , 2022, 74, 1376-1378.	0.9	1
5	Assessment of Outliers in Alloy Datasets Using Unsupervised Techniques. <i>Jom</i> , 2022, 74, 2846-2859.	0.9	3
6	Formation of multicomponent alloy particles in doped ceria under I ²⁺ ion irradiation and thermal annealing. <i>Journal of Nuclear Materials</i> , 2021, 545, 152638.	1.3	0
7	A machine learning aided interpretable model for rupture strength prediction in Fe-based martensitic and austenitic alloys. <i>Scientific Reports</i> , 2021, 11, 5466.	1.6	19
8	Machine learning augmented predictive and generative model for rupture life in ferritic and austenitic steels. <i>Npj Materials Degradation</i> , 2021, 5, .	2.6	23
9	Machine learning assisted prediction of the Young's modulus of compositionally complex alloys. <i>Scientific Reports</i> , 2021, 11, 17149.	1.6	38
10	A microstructure-based modeling approach to predict the mechanical properties of Zr alloy with hydride precipitates. <i>Computational Materials Science</i> , 2021, 197, 110654.	1.4	10
11	Incorporating Historical Data and Past Analyses for Improved Tensile Property Prediction of 9% Cr Steel. <i>Minerals, Metals and Materials Series</i> , 2021, , 461-472.	0.3	0
12	Data Science Techniques, Assumptions, and Challenges in Alloy Clustering and Property Prediction. <i>Journal of Materials Engineering and Performance</i> , 2021, 30, 823-838.	1.2	3
13	Energy-Dispersive X-ray Spectroscopy and Atom-probe Tomography Data Quantifying Component-Ratios of Multicomponent Nano-Precipitates in Ion-Irradiated Ceria. <i>Data in Brief</i> , 2021, 39, 107460.	0.5	0
14	Data Assessment Method to Support the Development of Creep-Resistant Alloys. <i>Integrating Materials and Manufacturing Innovation</i> , 2020, 9, 89-102.	1.2	6
15	A new non-diffusional gas bubble production route in used nuclear fuel: implications for fission gas release, cladding corrosion, and next generation fuel design. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 6086-6099.	1.3	3
16	Interatomic Potentials for Nuclear Materials. , 2020, , 2141-2159.		2
17	Data-driven glass/ceramic science research: Insights from the glass and ceramic and data science/informatics communities. <i>Journal of the American Ceramic Society</i> , 2019, 102, 6385-6406.	1.9	20
18	Hexagonal close-packed high-entropy alloy formation under extreme processing conditions. <i>Journal of Materials Research</i> , 2019, 34, 709-719.	1.2	7

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19	Highly Selective Supported Graphene Oxide Membranes for Water-Ethanol Separation. Scientific Reports, 2019, 9, 2251.	1.6	22
20	Role of interfaces in damage process of irradiated lithium aluminate nanocrystals. Journal of the American Ceramic Society, 2019, 102, 1982-1993.	1.9	7
21	In Situ Study of Particle Precipitation in Metal-Doped CeO ₂ during Thermal Treatment and Ion Irradiation for Emulation of Irradiating Fuels. Journal of Physical Chemistry C, 2019, 123, 2591-2601.	1.5	16
22	Unit mechanisms of fission gas release: Current understanding and future needs. Journal of Nuclear Materials, 2018, 504, 300-317.	1.3	80
23	Interatomic Potentials for Nuclear Materials. , 2018, , 1-19.		0
24	First principles investigation of the structural and bonding properties of hydrated actinide (IV) oxalates, An(C ₂ O ₄) ₂ ·6H ₂ O (An = U, Pu). Computational Materials Science, 2018, 153, 146-152.	1.4	7
25	Preliminary Evaluation of the DUSTRAN Modeling Suite for Modeling Atmospheric Chloride Transport. Air Quality, Atmosphere and Health, 2017, 10, 25-31.	1.5	1
26	Molecular Dynamics Simulation of Fission Fragment Damage in Nuclear Fuel and Surrogate Material. MRS Advances, 2017, 2, 1225-1230.	0.5	9
27	Low energy ion-solid interactions and chemistry effects in a series of pyrochlores. Journal of the American Ceramic Society, 2017, 100, 3132-3144.	1.9	7
28	Energy penalty for excess baggage. Nature Nanotechnology, 2017, 12, 500-501.	15.6	28
29	Insights on Amorphization of Lithium Aluminate from Atomistic Simulation. Journal of Physical Chemistry C, 2017, 121, 7635-7642.	1.5	17
30	Nanoparticle Precipitation in Irradiated and Annealed Ceria Doped with Metals for Emulation of Spent Fuels. Journal of Physical Chemistry C, 2017, 121, 22465-22477.	1.5	6
31	Molecular dynamics simulation of low-energy recoil events in titanate pyrochlores. RSC Advances, 2017, 7, 35403-35410.	1.7	6
32	Molecular dynamics simulation of the structural, elastic, and thermal properties of pyrochlores. RSC Advances, 2016, 6, 41410-41419.	1.7	25
33	Graphene oxide membranes with high permeability and selectivity for dehumidification of air. Carbon, 2016, 106, 164-170.	5.4	54
34	Molecular Dynamics Simulations Reveal that Water Diffusion between Graphene Oxide Layers is Slow. Scientific Reports, 2016, 6, 29484.	1.6	124
35	Characterization of swift heavy ion irradiation damage in ceria. Journal of Materials Research, 2015, 30, 1473-1484.	1.2	29
36	Advances in understanding of swift heavy-ion tracks in complex ceramics. Current Opinion in Solid State and Materials Science, 2015, 19, 39-48.	5.6	66

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37	Ion tracks and microstructures in barium titanate irradiated with swift heavy ions: A combined experimental and computational study. <i>Acta Materialia</i> , 2013, 61, 7904-7916.	3.8	18
38	Ab Initio Molecular Dynamics Simulation of Proton Hopping in a Model Polymer Membrane. <i>Journal of Physical Chemistry B</i> , 2013, 117, 16522-16529.	1.2	50
39	Role of cation choice in the radiation tolerance of pyrochlores. <i>RSC Advances</i> , 2013, 3, 2901.	1.7	19
40	Improved zircon fission-track annealing model based on reevaluation of annealing data. <i>Physics and Chemistry of Minerals</i> , 2013, 40, 93-106.	0.3	17
41	Molecular modeling of the morphology and transport properties of two direct methanol fuel cell membranes: Phenylated sulfonated poly(ether ether ketone ketone) versus Nafion. <i>Journal of Materials Research</i> , 2012, 27, 1927-1938.	1.2	6
42	Insight from molecular modelling: does the polymer side chain length matter for transport properties of perfluorosulfonic acid membranes?. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 11281.	1.3	51
43	Radiation-Induced Reduction of Ceria in Single and Polycrystalline Thin Films. <i>Journal of Physical Chemistry C</i> , 2012, 116, 361-366.	1.5	26
44	First-principles calculations of the electronic structure, phase transition and properties of ZrSiO ₄ polymorphs. <i>Computational and Theoretical Chemistry</i> , 2012, 987, 62-70.	1.1	23
45	Ab initio study of defect properties in YPO ₄ . <i>Computational Materials Science</i> , 2012, 54, 170-175.	1.4	10
46	Modeling the Nanophase Structural Dynamics of Phenylated Sulfonated Poly Ether Ether Ketone Ketone (Ph-SPEEKK) Membranes As a Function of Hydration. <i>Journal of Physical Chemistry B</i> , 2011, 115, 1817-1824.	1.2	15
47	Atomistic Simulations of Perfluoro Phosphonic and Phosphinic Acid Membranes and Comparisons to Nafion. <i>Journal of Physical Chemistry B</i> , 2011, 115, 2959-2969.	1.2	14
48	Stabilization Mechanisms of LaFeO ₃ (010) Surfaces Determined with First Principles Calculations. <i>Journal of the American Ceramic Society</i> , 2011, 94, 1931-1939.	1.9	18
49	Integrated experimental and modeling study of the ionic conductivity of samaria-doped ceria thin films. <i>Solid State Ionics</i> , 2011, 204-205, 13-19.	1.3	18
50	Molecular dynamics simulation of Xe bubble nucleation in nanocrystalline UO ₂ nuclear fuel. <i>Journal of Nuclear Materials</i> , 2011, 419, 140-144.	1.3	27
51	Molecular structure and transport dynamics in perfluoro sulfonyl imide membranes. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 234106.	0.7	8
52	Paramagnetic defects in electron-irradiated yttria-stabilized zirconia: Effect of yttria content. <i>Journal of Applied Physics</i> , 2011, 110, .	1.1	38
53	Simulation of collision cascades and thermal spikes in ceramics. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2010, 268, 2857-2862.	0.6	17
54	Integrated experimental and modeling study of ionic conductivity of scandia-stabilized zirconia thin films. <i>Solid State Ionics</i> , 2010, 181, 367-371.	1.3	9

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55	Application of the phase-field method in predicting gas bubble microstructure evolution in nuclear fuels. <i>International Journal of Materials Research</i> , 2010, 101, 515-522.	0.1	15
56	Atomistic Simulation of Water Percolation and Proton Hopping in Nafion Fuel Cell Membrane. <i>Journal of Physical Chemistry B</i> , 2010, 114, 13681-13690.	1.2	125
57	Structure and Dynamics of <i>N,N</i> -Diethyl- <i>N</i> -methylammonium Triflate Ionic Liquid, Neat and with Water, from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12764-12774.	1.1	58
58	Nanoscale phase transitions under extreme conditions within an ion track. <i>Journal of Materials Research</i> , 2010, 25, 1344-1351.	1.2	87
59	Ab Initio Study of Hydration and Proton Dissociation in Ionomer Membranes. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6904-6912.	1.1	33
60	Modeling and simulation of nuclear fuel materials. <i>Energy and Environmental Science</i> , 2010, 3, 1406.	15.6	80
61	Atomistic simulation of track formation by energetic recoils in zircon. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 395008.	0.7	21
62	Radiation tolerance of ceramics – insights from atomistic simulation of damage accumulation in pyrochlores. <i>Energy and Environmental Science</i> , 2010, 3, 1551.	15.6	59
63	Radiation damage evolution in ceramics. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2009, 267, 3017-3021.	0.6	25
64	Molecular-dynamics simulation of threshold displacement energies in zircon. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2009, 267, 3431-3436.	0.6	31
65	Energetic recoils in UO ₂ simulated using five different potentials. <i>Journal of Chemical Physics</i> , 2009, 130, 174502.	1.2	52
66	First-principles study of defects and phase transition in UO ₂ . <i>Journal of Physics Condensed Matter</i> , 2009, 21, 435401.	0.7	71
67	Unified interatomic potential for zircon, zirconia and silica systems. <i>Journal of Materials Chemistry</i> , 2009, 19, 3923.	6.7	38
68	Defect interactions and ionic transport in scandia stabilized zirconia. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 5506.	1.3	23
69	Recent developments in proton exchange membranes for fuel cells. <i>Energy and Environmental Science</i> , 2008, 1, 101.	15.6	462
70	Electron-Hole Pairs Created by Photons and Intrinsic Properties in Detector Materials. <i>IEEE Transactions on Nuclear Science</i> , 2008, 55, 1079-1085.	1.2	20
71	Dynamic annealing of defects in irradiated zirconia-based ceramics. <i>Journal of Materials Research</i> , 2008, 23, 593-597.	1.2	32
72	Atomistic Simulations of Hydrated Nafion and Temperature Effects on Hydronium Ion Mobility. <i>Journal of Physical Chemistry B</i> , 2007, 111, 7234-7244.	1.2	212

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73	Atomistic Simulation of Nafion Membrane: I. Effect of Hydration on Membrane Nanostructure. Journal of Physical Chemistry B, 2007, 111, 8069-8079.	1.2	220
74	Atomistic Simulation of Nafion Membrane. 2. Dynamics of Water Molecules and Hydronium Ions. Journal of Physical Chemistry B, 2007, 111, 13006-13013.	1.2	163
75	A fast screening technique to evaluate detector response. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2007, 579, 108-112.	0.7	9
76	Atomistic simulations of epitaxial recrystallization in 4H-SiC along the [0001] direction. Nuclear Instruments & Methods in Physics Research B, 2007, 255, 136-140.	0.6	3
77	Molecular dynamics simulation of amorphization in forsterite by cosmic rays. Nuclear Instruments & Methods in Physics Research B, 2007, 255, 172-176.	0.6	21
78	Atomistic modeling of amorphous silicon carbide using a bond-order potential. Nuclear Instruments & Methods in Physics Research B, 2007, 255, 130-135.	0.6	20
79	Gamma-ray interaction in Ge: A Monte Carlo simulation. Nuclear Instruments & Methods in Physics Research B, 2007, 255, 286-290.	0.6	30
80	Radiation effects in a model ceramic for nuclear waste disposal. Jom, 2007, 59, 32-35.	0.9	5
81	Monte Carlo method for simulating β -ray interaction with materials: A case study on Si. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2007, 579, 292-296.	0.7	33
82	Model of plasmon decay for electron cascade simulation. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2007, 579, 454-457.	0.7	4
83	Development of partial-charge potential for GaN. Nuclear Instruments & Methods in Physics Research B, 2006, 250, 50-53.	0.6	4
84	Atomistic simulation of collision cascades in zircon. Nuclear Instruments & Methods in Physics Research B, 2006, 250, 46-49.	0.6	5
85	Characterization of energy conservation in primary knock-on atom cascades: Ballistic phase effects on variable time steps. Nuclear Instruments & Methods in Physics Research B, 2006, 250, 6-11.	0.6	1
86	Computer simulation of defects and oxygen transport in yttria-stabilized zirconia. Solid State Ionics, 2006, 177, 1251-1258.	1.3	135
87	Short- and medium-range structure of amorphous zircon from molecular dynamics simulations. Physical Review B, 2006, 74, .	1.1	29
88	Signal variance in gamma-ray detectors—A review. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2006, 565, 637-649.	0.7	148
89	Atomic-level simulation of epitaxial recrystallization and phase transformation in SiC. Journal of Materials Research, 2006, 21, 1420-1426.	1.2	9
90	Molecular dynamics simulation of energetic uranium recoil damage in zircon. Molecular Simulation, 2006, 32, 1069-1077.	0.9	35

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91	Excess kinetic energy dissipation in materials. Nuclear Instruments & Methods in Physics Research B, 2005, 228, 274-281.	0.6	9
92	Annealing simulations of nano-sized amorphous structures in SiC. Nuclear Instruments & Methods in Physics Research B, 2005, 228, 282-287.	0.6	9
93	Molecular dynamics simulation of defect production in collision cascades in zircon. Nuclear Instruments & Methods in Physics Research B, 2005, 228, 299-303.	0.6	22
94	Threshold displacement energies in rutile TiO ₂ : A molecular dynamics simulation study. Nuclear Instruments & Methods in Physics Research B, 2005, 239, 191-201.	0.6	53
95	Defects and Ion-Solid Interactions in Silicon Carbide. Materials Science Forum, 2005, 475-479, 1345-1350.	0.3	0
96	Insights into the radiation response of pyrochlores from calculations of threshold displacement events. Journal of Applied Physics, 2005, 98, 086110.	1.1	40
97	Molecular dynamics simulation of disordered zircon. Physical Review B, 2004, 69, .	1.1	38
98	Ion-beam induced defects and nanoscale amorphous clusters in silicon carbide. Nuclear Instruments & Methods in Physics Research B, 2004, 216, 25-35.	0.6	35
99	Damage accumulation and amorphization in samarium titanate pyrochlore. Nuclear Instruments & Methods in Physics Research B, 2004, 218, 89-94.	0.6	20
100	The efficiency of damage production in silicon carbide. Nuclear Instruments & Methods in Physics Research B, 2004, 218, 68-73.	0.6	28
101	Damage evolution on Sm and O sublattices in Au-implanted samarium titanate pyrochlore. Journal of Applied Physics, 2004, 95, 2866-2872.	1.1	37
102	Amorphization of silicon carbide by carbon displacement. Applied Physics Letters, 2004, 84, 3909-3911.	1.5	36
103	Strong quantum confinement effects in polymer-based PbS nanostructures prepared by ion-exchange method. Materials Letters, 2004, 58, 1223-1226.	1.3	45
104	Experimental and Computational Studies of Ion-Solid Interactions in Silicon Carbide. Materials Research Society Symposia Proceedings, 2003, 792, 39.	0.1	3
105	Experimental and Computer Simulation Studies of Defects and Ion-Solid Interactions in Silicon Carbide. Materials Science Forum, 2002, 389-393, 875-878.	0.3	1
106	Ion-solids interactions and defects in silicon carbide. Nuclear Instruments & Methods in Physics Research B, 2002, 190, 261-265.	0.6	7
107	Fractal nature of crystalline-crystalline interface in CuInSe ₂ thin films. Materials Research Bulletin, 2002, 37, 1475-1480.	2.7	5
108	Defect production, multiple ion-solids interactions and amorphization in SiC. Nuclear Instruments & Methods in Physics Research B, 2002, 191, 487-496.	0.6	104

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109	Heavy-ion irradiation effects on structures and acid dissolution of pyrochlores. Journal of Nuclear Materials, 2001, 288, 208-216.	1.3	111
110	Substructural recovery in a cold worked Ti-modified austenitic stainless steel during high temperature low cycle fatigue. International Journal of Fatigue, 2001, 23, 789-797.	2.8	26
111	Atomic-scale simulation of displacement cascades and amorphization in $\hat{\Gamma}^2$ -SiC. Nuclear Instruments & Methods in Physics Research B, 2001, 180, 176-186.	0.6	46
112	Atomic scale simulation of defect production in irradiated 3C-SiC. Journal of Applied Physics, 2001, 90, 2303-2309.	1.1	211
113	Displacement energy surface in 3C and 6H SiC. Journal of Nuclear Materials, 2000, 278, 258-265.	1.3	207
114	Native vacancy migrations in zircon. Journal of Nuclear Materials, 1999, 273, 164-170.	1.3	34
115	Effects of Cation Disorder on Oxygen Vacancy Migration in Gd ₂ Ti ₂ O ₇ . , 1999, 3, 409-424.		80
116	The effect of temperature on the low cycle fatigue properties of a 15Cr-15Ni, Ti modified austenitic stainless steel. Scripta Materialia, 1999, 41, 921-927.	2.6	16
117	Computer simulation of displacement energies for several ceramic materials. Nuclear Instruments & Methods in Physics Research B, 1998, 141, 94-98.	0.6	55
118	Computer simulation of a 10 keV Si displacement cascade in SiC. Nuclear Instruments & Methods in Physics Research B, 1998, 141, 118-122.	0.6	95
119	Displacement threshold energies in $\hat{\Gamma}^2$ -SiC. Journal of Nuclear Materials, 1998, 253, 47-52.	1.3	151
120	Effects of ionizing radiation in ceramics. Journal of Nuclear Materials, 1998, 253, 113-119.	1.3	26
121	A comparison between the irradiation damage response of spinel and zirconia due to Xe ion bombardment. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 1998, 253, 78-85.	2.6	33
122	Radiation response of FeTiO ₃ , MgTiO ₃ , and $\hat{\Gamma}^{\pm}$ -Al ₂ O ₃ . Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 1998, 253, 131-134.	2.6	14
123	Radiation-induced phase transformations in MgAl ₂ O ₄ spinel. Journal of Materials Research, 1997, 12, 1766-1770.	1.2	22
124	Elastic instability in ion-beam-irradiated magnesium aluminate spinel. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1997, 75, 793-801.	0.6	8
125	Structure and mechanical properties of irradiated magnesium aluminate spinel. Journal of Nuclear Materials, 1996, 232, 59-64.	1.3	48
126	Atomistic study of defect, metastable and 'amorphous' structures of MgAl ₂ O ₄ . Philosophical Magazine Letters, 1996, 73, 51-62.	0.5	43

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127	The irradiation damage response of MgO · 3Al ₂ O ₃ spinel single crystal under high-fluence ion-irradiation. Nuclear Instruments & Methods in Physics Research B, 1995, 106, 573-578.	0.6	20
128	Structure of the metastable state in ion-irradiated magnesio-aluminate spinel. Philosophical Magazine Letters, 1995, 72, 155-161.	0.5	30
129	Atomistic simulation of radiation-induced amorphization of the ordered compound NiZr. Journal of Alloys and Compounds, 1993, 194, 447-454.	2.8	24
130	Radiation-induced crystalline-to-amorphous transition in intermetallic compounds of the Cu-Ti alloy system. Journal of Alloys and Compounds, 1993, 194, 429-437.	2.8	18
131	Molecular-dynamics simulation of electron-irradiation-induced amorphization of NiZr ₂ . Physical Review B, 1993, 48, 42-51.	1.1	55