Ram Devanathan

List of Publications by Year
in descending order

131 papers	5,254 citations	101543 36 h-index	98798 67 g-index
137 all docs	137 docs citations	137 times ranked	4440 citing authors

#	Article	IF	Citations
1	Recent developments in proton exchange membranes for fuel cells. Energy and Environmental Science, 2008, 1, 101.	30.8	462
2	Atomistic Simulation of Nafion Membrane:Â I. Effect of Hydration on Membrane Nanostructure. Journal of Physical Chemistry B, 2007, 111, 8069-8079.	2.6	220
3	Atomistic Simulations of Hydrated Nafion and Temperature Effects on Hydronium Ion Mobility. Journal of Physical Chemistry B, 2007, 111, 7234-7244.	2.6	212
4	Atomic scale simulation of defect production in irradiated 3C-SiC. Journal of Applied Physics, 2001, 90, 2303-2309.	2.5	211
5	Displacement energy surface in 3C and 6H SiC. Journal of Nuclear Materials, 2000, 278, 258-265.	2.7	207
6	Atomistic Simulation of Nafion Membrane. 2. Dynamics of Water Molecules and Hydronium Ions. Journal of Physical Chemistry B, 2007, 111, 13006-13013.	2.6	163
7	Displacement threshold energies in Î²-SiC. Journal of Nuclear Materials, 1998, 253, 47-52.	2.7	151
8	Signal variance in gamma-ray detectorsâ€”A review. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2006, 565, 637-649.	1.6	148
9	Computer simulation of defects and oxygen transport in yttria-stabilized zirconia. Solid State Ionics, 2006, 177, 1251-1258.	2.7	135
10	Atomistic Simulation of Water Percolation and Proton Hopping in Nafion Fuel Cell Membrane. Journal of Physical Chemistry B, 2010, 114, 13681-13690.	2.6	125
11	Molecular Dynamics Simulations Reveal that Water Diffusion between Graphene Oxide Layers is Slow. Scientific Reports, 2016, 6, 29484.	3.3	124
12	Heavy-ion irradiation effects on structures and acid dissolution of pyrochlores. Journal of Nuclear Materials, 2001, 288, 208-216.	2.7	111
13	Defect production, multiple ionâ€“solid interactions and amorphization in SiC. Nuclear Instruments & Methods in Physics Research B, 2002, 191, 487-496.	1.4	104
14	Computer simulation of a 10 keV Si displacement cascade in SiC. Nuclear Instruments & Methods in Physics Research B, 1998, 141, 118-122.	1.4	95
15	Nanoscale phase transitions under extreme conditions within an ion track. Journal of Materials Research, 2010, 25, 1344-1351.	2.6	87
16	Effects of Cation Disorder on Oxygen Vacancy Migration in Gd2Ti2O7. , 1999, 3, 409-424.		80
17	Modeling and simulation of nuclear fuel materials. Energy and Environmental Science, 2010, 3, 1406.	30.8	80
18	Unit mechanisms of fission gas release: Current understanding and future needs. Journal of Nuclear Materials, 2018, 504, 300-317.	2.7	80

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19	First-principles study of defects and phase transition in UO₂. Journal of Physics Condensed Matter, 2009, 21, 435401.	1.8	71
20	Advances in understanding of swift heavy-ion tracks in complex ceramics. Current Opinion in Solid State and Materials Science, 2015, 19, 39-48.	11.5	66
21	Radiation tolerance of ceramicsâ€"insights from atomistic simulation of damage accumulation in pyrochlores. Energy and Environmental Science, 2010, 3, 1551.	30.8	59
22	Structure and Dynamics of N,N-Diethyl-N-methylammonium Triflate Ionic Liquid, Neat and with Water, from Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2010, 114, 12764-12774.	2.5	58
23	Molecular-dynamics simulation of electron-irradiation-induced amorphization ofNiZr2. Physical Review B, 1993, 48, 42-51.	3.2	55
24	Computer simulation of displacement energies for several ceramic materials. Nuclear Instruments & Methods in Physics Research B, 1998, 141, 94-98.	1.4	55
25	Graphene oxide membranes with high permeability and selectivity for dehumidification of air. Carbon, 2016, 106, 164-170.	10.3	54
26	Threshold displacement energies in rutile TiO2: A molecular dynamics simulation study. Nuclear Instruments & Methods in Physics Research B, 2005, 239, 191-201.	1.4	53
27	Energetic recoils in UO2 simulated using five different potentials. Journal of Chemical Physics, 2009, 130, 174502.	3.0	52
28	Insight from molecular modelling: does the polymer side chain length matter for transport properties of perfluorosulfonic acid membranes?. Physical Chemistry Chemical Physics, 2012, 14, 11281.	2.8	51
29	Ab Initio Molecular Dynamics Simulation of Proton Hopping in a Model Polymer Membrane. Journal of Physical Chemistry B, 2013, 117, 16522-16529.	2.6	50
30	Structure and mechanical properties of irradiated magnesium aluminate spinel. Journal of Nuclear Materials, 1996, 232, 59-64.	2.7	48
31	Atomic-scale simulation of displacement cascades and amorphization in Î²-SiC. Nuclear Instruments & Methods in Physics Research B, 2001, 180, 176-186.	1.4	46
32	Strong quantum confinement effects in polymer-based PbS nanostructures prepared by ion-exchange method. Materials Letters, 2004, 58, 1223-1226.	2.6	45
33	Atomistic study of defect, metastable and 'amorphous' structures of MgAl204. Philosophical Magazine Letters, 1996, 73, 51-62.	1.2	43
34	Insights into the radiation response of pyrochlores from calculations of threshold displacement events. Journal of Applied Physics, 2005, 98, 086110.	2.5	40
35	Molecular dynamics simulation of disordered zircon. Physical Review B, 2004, 69, .	3.2	38
36	Unified interatomic potential for zircon, zirconia and silica systems. Journal of Materials Chemistry, 2009, 19, 3923.	6.7	38

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37	Paramagnetic defects in electron-irradiated yttria-stabilized zirconia: Effect of yttria content. Journal of Applied Physics, 2011, 110, .	2.5	38
38	Machine learning assisted prediction of the Youngâ€™s modulus of compositionally complex alloys. Scientific Reports, 2021, 11, 17149.	3.3	38
39	Damage evolution on Sm and O sublattices in Au-implanted samarium titanate pyrochlore. Journal of Applied Physics, 2004, 95, 2866-2872.	2.5	37
40	Amorphization of silicon carbide by carbon displacement. Applied Physics Letters, 2004, 84, 3909-3911.	3.3	36
41	Ion-beam induced defects and nanoscale amorphous clusters in silicon carbide. Nuclear Instruments & Methods in Physics Research B, 2004, 216, 25-35.	1.4	35
42	Molecular dynamics simulation of energetic uranium recoil damage in zircon. Molecular Simulation, 2006, 32, 1069-1077.	2.0	35
43	Native vacancy migrations in zircon. Journal of Nuclear Materials, 1999, 273, 164-170.	2.7	34
44	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.	5.6	33
45	Monte Carlo method for simulating Î³-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.	1.6	33
46	Ab Initio Study of Hydration and Proton Dissociation in Ionomer Membranes. Journal of Physical Chemistry A, 2010, 114, 6904-6912.	2.5	33
47	Dynamic annealing of defects in irradiated zirconia-based ceramics. Journal of Materials Research, 2008, 23, 593-597.	2.6	32
48	Molecular-dynamics simulation of threshold displacement energies in zircon. Nuclear Instruments & Methods in Physics Research B, 2009, 267, 3431-3436.	1.4	31
49	Structure of the metastable state in ion-irradiated magnesio-aluminate spinel. Philosophical Magazine Letters, 1995, 72, 155-161.	1.2	30
50	Gamma-ray interaction in Ge: A Monte Carlo simulation. Nuclear Instruments & Methods in Physics Research B, 2007, 255, 286-290.	1.4	30
51	Short- and medium-range structure of amorphous zircon from molecular dynamics simulations. Physical Review B, 2006, 74, .	3.2	29
52	Characterization of swift heavy ion irradiation damage in ceria. Journal of Materials Research, 2015, 30, 1473-1484.	2.6	29
53	Machine-learning-guided descriptor selection for predicting corrosion resistance in multi-principal element alloys. Npj Materials Degradation, 2022, 6, .	5.8	29
54	The efficiency of damage production in silicon carbide. Nuclear Instruments & Methods in Physics Research B, 2004, 218, 68-73.	1.4	28

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55	Energy penalty for excess baggage. Nature Nanotechnology, 2017, 12, 500-501.	31.5	28
56	Molecular dynamics simulation of Xe bubble nucleation in nanocrystalline UO2 nuclear fuel. Journal of Nuclear Materials, 2011, 419, 140-144.	2.7	27
57	Effects of ionizing radiation in ceramics. Journal of Nuclear Materials, 1998, 253, 113-119.	2.7	26
58	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.	5.7	26
59	Radiation-Induced Reduction of Ceria in Single and Polycrystalline Thin Films. Journal of Physical Chemistry C, 2012, 116, 361-366.	3.1	26
60	Radiation damage evolution in ceramics. Nuclear Instruments & Methods in Physics Research B, 2009, 267, 3017-3021.	1.4	25
61	Molecular dynamics simulation of the structural, elastic, and thermal properties of pyrochlores. RSC Advances, 2016, 6, 41410-41419.	3.6	25
62	Atomistic simulation of radiation-induced amorphization of the ordered compound NiZr. Journal of Alloys and Compounds, 1993, 194, 447-454.	5.5	24
63	Defect interactions and ionic transport in scandia stabilized zirconia. Physical Chemistry Chemical Physics, 2009, 11, 5506.	2.8	23
64	First-principles calculations of the electronic structure, phase transition and properties of ZrSiO4 polymorphs. Computational and Theoretical Chemistry, 2012, 987, 62-70.	2.5	23
65	Machine learning augmented predictive and generative model for rupture life in ferritic and austenitic steels. Npj Materials Degradation, 2021, 5, .	5.8	23
66	Radiation-induced phase transformations in MgAl₂O₄ spinel. Journal of Materials Research, 1997, 12, 1766-1770.	2.6	22
67	Molecular dynamics simulation of defect production in collision cascades in zircon. Nuclear Instruments & Methods in Physics Research B, 2005, 228, 299-303.	1.4	22
68	Highly Selective Supported Graphene Oxide Membranes for Water-Ethanol Separation. Scientific Reports, 2019, 9, 2251.	3.3	22
69	Molecular dynamics simulation of amorphization in forsterite by cosmic rays. Nuclear Instruments & Methods in Physics Research B, 2007, 255, 172-176.	1.4	21
70	Atomistic simulation of track formation by energetic recoils in zircon. Journal of Physics Condensed Matter, 2010, 22, 395008.	1.8	21
71	The irradiation damage response of MgO Â· 3Al2O3 spinel single crystal under high-fluence ion-irradiation. Nuclear Instruments & Methods in Physics Research B, 1995, 106, 573-578.	1.4	20
72	Damage accumulation and amorphization in samarium titanate pyrochlore. Nuclear Instruments & Methods in Physics Research B, 2004, 218, 89-94.	1.4	20

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73	Atomistic modeling of amorphous silicon carbide using a bond-order potential. Nuclear Instruments & Methods in Physics Research B, 2007, 255, 130-135.	1.4	20
74	Electron-Hole Pairs Created by Photons and Intrinsic Properties in Detector Materials. IEEE Transactions on Nuclear Science, 2008, 55, 1079-1085.	2.0	20
75	Dataâ€driven glass/ceramic science research: Insights from the glass and ceramic and data science/informatics communities. Journal of the American Ceramic Society, 2019, 102, 6385-6406.	3.8	20
76	Role of cation choice in the radiation tolerance of pyrochlores. RSC Advances, 2013, 3, 2901.	3.6	19
77	A machine learning aided interpretable model for rupture strength prediction in Fe-based martensitic and austenitic alloys. Scientific Reports, 2021, 11, 5466.	3.3	19
78	Radiation-induced crystalline-to-amorphous transition in intermetallic compounds of the Cuî—¸Ti alloy system. Journal of Alloys and Compounds, 1993, 194, 429-437.	5.5	18
79	Stabilization Mechanisms of LaFeO3 (010) Surfaces Determined with First Principles Calculations. Journal of the American Ceramic Society, 2011, 94, 1931-1939.	3.8	18
80	Integrated experimental and modeling study of the ionic conductivity of samaria-doped ceria thin films. Solid State Ionics, 2011, 204-205, 13-19.	2.7	18
81	Ion tracks and microstructures in barium titanate irradiated with swift heavy ions: A combined experimental and computational study. Acta Materialia, 2013, 61, 7904-7916.	7.9	18
82	Simulation of collision cascades and thermal spikes in ceramics. Nuclear Instruments & Methods in Physics Research B, 2010, 268, 2857-2862.	1.4	17
83	Improved zircon fission-track annealing model based on reevaluation of annealing data. Physics and Chemistry of Minerals, 2013, 40, 93-106.	0.8	17
84	Insights on Amorphization of Lithium Aluminate from Atomistic Simulation. Journal of Physical Chemistry C, 2017, 121, 7635-7642.	3.1	17
85	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.	5.2	16
86	In Situ Study of Particle Precipitation in Metal-Doped CeO₂ during Thermal Treatment and Ion Irradiation for Emulation of Irradiating Fuels. Journal of Physical Chemistry C, 2019, 123, 2591-2601.	3.1	16
87	Application of the phase-field method in predicting gas bubble microstructure evolution in nuclear fuels. International Journal of Materials Research, 2010, 101, 515-522.	0.3	15
88	Modeling the Nanophase Structural Dynamics of Phenylated Sulfonated Poly Ether Ether Ketone Ketone (Ph-SPEEKK) Membranes As a Function of Hydration. Journal of Physical Chemistry B, 2011, 115, 1817-1824.	2.6	15
89	Radiation response of FeTiO3, MgTiO3, and Î±-Al2O3. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 1998, 253, 131-134.	5.6	14
90	Atomistic Simulations of Perfluoro Phosphonic and Phosphinic Acid Membranes and Comparisons to Nafion. Journal of Physical Chemistry B, 2011, 115, 2959-2969.	2.6	14

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91	Grain-size effects on the deformation in nanocrystalline multi-principal element alloy. Materials Chemistry and Physics, 2022, 277, 125546.	4.0	14
92	Ab initio study of defect properties in YPO4. Computational Materials Science, 2012, 54, 170-175.	3.0	10
93	A microstructure-based modeling approach to predict the mechanical properties of Zr alloy with hydride precipitates. Computational Materials Science, 2021, 197, 110654.	3.0	10
94	Excess kinetic energy dissipation in materials. Nuclear Instruments & Methods in Physics Research B, 2005, 228, 274-281.	1.4	9
95	Annealing simulations of nano-sized amorphous structures in SiC. Nuclear Instruments & Methods in Physics Research B, 2005, 228, 282-287.	1.4	9
96	Atomic-level simulation of epitaxial recrystallization and phase transformation in SiC. Journal of Materials Research, 2006, 21, 1420-1426.	2.6	9
97	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.	1.6	9
98	Integrated experimental and modeling study of ionic conductivity of scandia-stabilized zirconia thin films. Solid State Ionics, 2010, 181, 367-371.	2.7	9
99	Molecular Dynamics Simulation of Fission Fragment Damage in Nuclear Fuel and Surrogate Material. MRS Advances, 2017, 2, 1225-1230.	0.9	9
100	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
101	Molecular structure and transport dynamics in perfluoro sulfonyl imide membranes. Journal of Physics Condensed Matter, 2011, 23, 234106.	1.8	8
102	Ionâ€“solid interactions and defects in silicon carbide. Nuclear Instruments & Methods in Physics Research B, 2002, 190, 261-265.	1.4	7
103	Low energy ionâ€solid interactions and chemistry effects in a series of pyrochlores. Journal of the American Ceramic Society, 2017, 100, 3132-3144.	3.8	7
104	First principles investigation of the structural and bonding properties of hydrated actinide (IV) oxalates, An(C2O4)2Â·6H2O (Anâ€¯=â€¯U, Pu). Computational Materials Science, 2018, 153, 146-152.	3.0	7
105	Hexagonal close-packed high-entropy alloy formation under extreme processing conditions. Journal of Materials Research, 2019, 34, 709-719.	2.6	7
106	Role of interfaces in damage process of irradiated lithium aluminate nanocrystals. Journal of the American Ceramic Society, 2019, 102, 1982-1993.	3.8	7
107	Molecular modeling of the morphology and transport properties of two direct methanol fuel cell membranes: Phenylated sulfonated poly(ether ether ketone ketone) versus Nafion. Journal of Materials Research, 2012, 27, 1927-1938.	2.6	6
108	Nanoparticle Precipitation in Irradiated and Annealed Ceria Doped with Metals for Emulation of Spent Fuels. Journal of Physical Chemistry C, 2017, 121, 22465-22477.	3.1	6

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109	Data Assessment Method to Support the Development of Creep-Resistant Alloys. Integrating Materials and Manufacturing Innovation, 2020, 9, 89-102.	2.6	6
110	Molecular dynamics simulation of low-energy recoil events in titanate pyrochlores. RSC Advances, 2017, 7, 35403-35410.	3.6	6
111	Fractal nature of crystallineâ€“crystalline interface in CuInSe2 thin films. Materials Research Bulletin, 2002, 37, 1475-1480.	5.2	5
112	Atomistic simulation of collision cascades in zircon. Nuclear Instruments & Methods in Physics Research B, 2006, 250, 46-49.	1.4	5
113	Radiation effects in a model ceramic for nuclear waste disposal. Jom, 2007, 59, 32-35.	1.9	5
114	Uncertainty quantification for Bayesian active learning in rupture life prediction of ferritic steels. Scientific Reports, 2022, 12, 2083.	3.3	5
115	Development of partial-charge potential for GaN. Nuclear Instruments & Methods in Physics Research B, 2006, 250, 50-53.	1.4	4
116	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.	1.6	4
117	Experimental and Computational Studies of Ion-Solid Interactions in Silicon Carbide. Materials Research Society Symposia Proceedings, 2003, 792, 39.	0.1	3
118	Atomistic simulations of epitaxial recrystallization in 4H-SiC along the [0001] direction. Nuclear Instruments & Methods in Physics Research B, 2007, 255, 136-140.	1.4	3
119	A new non-diffusional gas bubble production route in used nuclear fuel: implications for fission gas release, cladding corrosion, and next generation fuel design. Physical Chemistry Chemical Physics, 2020, 22, 6086-6099.	2.8	3
120	Data Science Techniques, Assumptions, and Challenges in Alloy Clustering and Property Prediction. Journal of Materials Engineering and Performance, 2021, 30, 823-838.	2.5	3
121	Assessment of Outliers in Alloy Datasets Using Unsupervised Techniques. Jom, 2022, 74, 2846-2859.	1.9	3
122	Interatomic Potentials for Nuclear Materials. , 2020, , 2141-2159.		2
123	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
124	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.	1.4	1
125	Preliminary Evaluation of the DUSTRAN Modeling Suite for Modeling Atmospheric Chloride Transport. Air Quality, Atmosphere and Health, 2017, 10, 25-31.	3.3	1
126	Computational Design of Alloys for Energy Technologies. Jom, 2022, 74, 1376-1378.	1.9	1

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127	Defects and Ion-Solid Interactions in Silicon Carbide. Materials Science Forum, 2005, 475-479, 1345-1350.	0.3	0
128	Interatomic Potentials for Nuclear Materials. , 2018, , 1-19.		0
129	Formation of multicomponent alloy particles in doped ceria under I2+ ion irradiation and thermal annealing. Journal of Nuclear Materials, 2021, 545, 152638.	2.7	0
130	Incorporating Historical Data and Past Analyses for Improved Tensile Property Prediction of 9% Cr Steel. Minerals, Metals and Materials Series, 2021, , 461-472.	0.4	0
131	Energy-Dispersive X-ray Spectroscopy and Atom-probe Tomography Data Quantifying Component-Ratios of Multicomponent Nano-Precipitates in Ion-Irradiated Ceria. Data in Brief, 2021, 39, 107460.	1.0	0