

Patrick A Burr

List of Publications by Year in descending order

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59
all docs

59
docs citations

59
times ranked

1155
citing authors

#	ARTICLE	IF	CITATIONS
1	On the microstructure and high-temperature stability of nano-grained Zircaloy-4. Scripta Materialia, 2022, 210, 114410.	2.6	0
2	Molecular dynamic simulation on temperature evolution of SiC under directional microwave radiation. Journal of Physics Condensed Matter, 2022, 34, 195701.	0.7	1
3	Hydrogen solubility in Zr-Nb alloys. Scripta Materialia, 2022, 214, 114652.	2.6	6
4	A DFT study to determine the structure and composition of μ -W ₂ B ₅ x. Journal of Alloys and Compounds, 2022, 911, 164962.	2.8	5
5	Designing 3d metal oxides: selecting optimal density functionals for strongly correlated materials. Physical Chemistry Chemical Physics, 2022, 24, 14119-14139.	1.3	4
6	Structural and phase evolution in U ₃ Si ₂ during steam corrosion. Corrosion Science, 2022, 204, 110373.	3.0	3
7	Design considerations for high entropy alloys in advanced nuclear applications. Journal of Nuclear Materials, 2022, 567, 153814.	1.3	36
8	A molecular dynamics method to identify the liquidus and solidus in a binary phase diagram. Computational Materials Science, 2021, 186, 110016.	1.4	7
9	The predicted shapes of voids and Xe bubbles in UO_2 . Journal of Nuclear Materials, 2021, 543, 152622.	1.3	4
10	Intrinsic defect migration in Be ₁₂ Ti. Intermetallics, 2021, 128, 106937.	1.8	4
11	Atomistic Insights into Lithium Storage Mechanisms in Anatase, Rutile, and Amorphous TiO ₂ Electrodes. ACS Applied Materials & Interfaces, 2021, 13, 1791-1806.	4.0	32
12	Evidence of hydrogen trapping at second phase particles in zirconium alloys. Scientific Reports, 2021, 11, 4370.	1.6	9
13	Solubility and vacancy-mediated inter-diffusion in the Zr-Nb-Cr system. Journal of Nuclear Materials, 2021, 548, 152867.	1.3	5
14	Kinetics studies of thin film amorphous titanium niobium oxides for lithium ion battery anodes. Electrochimica Acta, 2021, 388, 138544.	2.6	2
15	Doped Nickel Oxide Carrier-Selective Contact for Silicon Solar Cells. IEEE Journal of Photovoltaics, 2021, 11, 1176-1187.	1.5	10
16	The speciation of niobium in the oxide layer of an irradiated Low-Tin ZIRLO nuclear material. Corrosion Science, 2021, 190, 109630.	3.0	5
17	Thermophysical properties of urania-zirconia (U,Zr)O ₂ mixed oxides by molecular dynamics. Journal of Nuclear Materials, 2020, 528, 151876.	1.3	3
18	Radiation-Induced Evolution of Tungsten Carbide in Fusion Reactors: Accommodation of Defect Clusters and Transmutation Elements. ACS Applied Energy Materials, 2020, 3, 868-878.	2.5	16

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19	Reduced Silicon Fragmentation in Lithium Ion Battery Anodes Using Electronic Doping Strategies. ACS Applied Energy Materials, 2020, 3, 1730-1741.	2.5	19
20	Fabrication strategies for high-rate TiO ₂ nanotube anodes for Li ion energy storage. Journal of Power Sources, 2020, 463, 228205.	4.0	16
21	predict the solidus and liquidus of mixed oxides $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mo} \text{stretchy="true"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{Th} \langle \text{mml:mtext} \rangle \langle \text{mml:mo} \rangle, \langle \text{mml:mo} \rangle \langle \text{mml:mtext} \rangle \text{U} \langle \text{mml:mtext} \rangle \langle \text{mml:mo} \rangle$	1.3	13
22	Diffusion mechanisms of Mo contamination in Si. Physical Review Materials, 2020, 4, .	0.9	2
23	PLuS Alliance Nuclear Engineering Online Course Exchange Program. , 2020, , .		0
24	Fundamental Point Defect Properties in Ceramics. , 2020, , 50-73.		0
25	Time domain modelling of concurrent insertion and capacitive storage using Laplace domain representations of impedance. Journal of Electroanalytical Chemistry, 2019, 850, 113379.	1.9	5
26	A review on the development of nuclear power reactors. Energy Procedia, 2019, 160, 459-466.	1.8	54
27	Understanding the importance of the energetics of Mn, Ni, Cu, Si and vacancy triplet clusters in bcc Fe. Journal of Applied Physics, 2019, 126, 115901.	1.1	12
28	Improving generation ramp rates of photovoltaic systems using module-based capacitive energy storage. Journal of Power Sources, 2019, 423, 227-235.	4.0	8
29	High-rate lithium ion energy storage to facilitate increased penetration of photovoltaic systems in electricity grids. MRS Energy & Sustainability, 2019, 6, 1.	1.3	10
30	Photovoltaic Power Generation with Module-Based Capacitive Energy Storage. , 2019, , .		0
31	Defect evolution in burnable absorber candidate material: Uranium diboride, UB ₂ . Journal of Nuclear Materials, 2019, 513, 45-55.	1.3	18
32	Formation and migration of point defects in tungsten carbide: Unveiling the sluggish bulk self-diffusivity of WC. Journal of the European Ceramic Society, 2019, 39, 165-172.	2.8	19
33	First-principles calculations of solute transport in zirconium: Vacancy-mediated diffusion with metastable states and interstitial diffusion. Physical Review Materials, 2019, 3, .	0.9	12
34	The formation and structure of Fe-Mn-Ni-Si solute clusters and G-phase precipitates in steels. Journal of Nuclear Materials, 2018, 505, 1-6.	1.3	31
35	Suitability of representative electrochemical energy storage technologies for ramp-rate control of photovoltaic power. Journal of Power Sources, 2018, 384, 396-407.	4.0	25
36	Evidence for Fast Lithium-Ion Diffusion and Charge-Transfer Reactions in Amorphous TiO _x Nanotubes: Insights for High-Rate Electrochemical Energy Storage. ACS Applied Materials & Interfaces, 2018, 10, 42513-42523.	4.0	28

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37	Extrinsic Defects in Crystalline MoO ₃ : Solubility and Effect on the Electronic Structure. Journal of Physical Chemistry C, 2018, 122, 27241-27249.	1.5	7
38	Anisotropy in the thermal expansion of uranium silicide measured by neutron diffraction. Journal of Nuclear Materials, 2018, 508, 516-520.	1.3	19
39	Density functional theory study of the magnetic moment of solute Mn in bcc Fe. Physical Review B, 2018, 98, .	1.1	14
40	DFT study of the hexagonal high-entropy alloy fission product system. Journal of Nuclear Materials, 2017, 488, 70-74.	1.3	18
41	Importance of elastic finite-size effects: Neutral defects in ionic compounds. Physical Review B, 2017, 96, .	1.1	22
42	Formation of intrinsic and silicon defects in MoO ₃ under varied oxygen partial pressure and temperature conditions: an ab initio DFT investigation. RSC Advances, 2017, 7, 53810-53821.	1.7	18
43	Experimental and DFT investigation of (Cr,Ti) ₃ AlC ₂ MAX phases stability. Materials Research Letters, 2017, 5, 144-157.	4.1	27
44	Defect processes in Be ₁₂ X (X=Ti, Mo, V, W). Nuclear Fusion, 2017, 57, 086049.	1.6	19
45	Solubility and partitioning of impurities in Be alloys. Journal of Alloys and Compounds, 2016, 688, 382-385.	2.8	4
46	Development of Xe and Kr empirical potentials for CeO ₂ , ThO ₂ , UO ₂ and PuO ₂ , combining DFT with high temperature MD. Journal of Physics Condensed Matter, 2016, 28, 405401.	0.7	29
47	Resolving the structure of TiBe ₁₂ . Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 277-280.	0.5	11
48	Synthesis and Oxidation Testing of <sc>MAX</sc> Phase Composites in the Cr-Ti-Al-C Quaternary System. Journal of the American Ceramic Society, 2016, 99, 682-690.	1.9	58
49	The influence of alloying elements on the corrosion of Zr alloys. Corrosion Science, 2016, 105, 36-43.	3.0	40
50	Structural stability and fission product behaviour in U ₃ Si. Journal of Nuclear Materials, 2015, 466, 739-744.	1.3	22
51	Crystal structure, thermodynamics, magnetism and disorder properties of Be-Fe-Al intermetallics. Journal of Alloys and Compounds, 2015, 639, 111-122.	2.8	11
52	Accommodation of tin in tetragonal ZrO ₂ . Journal of Applied Physics, 2015, 117, .	1.1	36
53	From solid solution to cluster formation of Fe and Cr in β -Zr. Journal of Nuclear Materials, 2015, 467, 320-331.	1.3	23
54	The thermodynamics of hydride precipitation: The importance of entropy, enthalpy and disorder. Acta Materialia, 2014, 79, 351-362.	3.8	59

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55	Peroxide defect formation in zirconate perovskites. Journal of Materials Chemistry A, 2014, 2, 15883-15888.	5.2	25
56	Hydrogen accommodation in Zr second phase particles: Implications for H pick-up and hydriding of Zircaloy-2 and Zircaloy-4. Corrosion Science, 2013, 69, 1-4.	3.0	43
57	Hydrogen solubility in zirconium intermetallic second phase particles. Journal of Nuclear Materials, 2013, 443, 502-506.	1.3	25
58	The stability of alloying additions in Zirconium. Journal of Nuclear Materials, 2013, 437, 122-129.	1.3	43