Tae Wook Heo

List of Publications by Year
in descending order

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Version: 2024-02-01

62 papers	1,964 citations	331670 21 h-index	254184 43 g-index
62 all docs	62 docs citations	62 times ranked	2085 citing authors

#	Article	IF	Citations
1	Nanostructured Metal Hydrides for Hydrogen Storage. Chemical Reviews, 2018, 118, 10775-10839.	47.7	461
2	Microstructural control in metal laser powder bed fusion additive manufacturing using laser beam shaping strategy. Acta Materialia, 2020, 184, 284-305.	7.9	192
3	Structural, Chemical, and Dynamical Frustration: Origins of Superionic Conductivity in closo-Borate Solid Electrolytes. Chemistry of Materials, 2017, 29, 9142-9153.	6.7	126
4	Understanding Ionic Conductivity Trends in Polyborane Solid Electrolytes from Ab Initio Molecular Dynamics. ACS Energy Letters, 2017, 2, 250-255.	17.4	75
5	Hierarchically Controlled Insideâ€Out Doping of Mg Nanocomposites for Moderate Temperature Hydrogen Storage. Advanced Functional Materials, 2017, 27, 1704316.	14.9	72
6	Toward an integrated computational system for describing the additive manufacturing process for metallic materials. Additive Manufacturing, 2014, 1-4, 52-63.	3.0	70
7	Phase-field modeling of displacive phase transformations in elastically anisotropic and inhomogeneous polycrystals. Acta Materialia, 2014, 76, 68-81.	7.9	66
8	A phase-field model of stress effect on grain boundary migration. Modelling and Simulation in Materials Science and Engineering, 2011, 19, 035002.	2.0	55
9	A phase field study of strain energy effects on soluteâ€“grain boundary interactions. Acta Materialia, 2011, 59, 7800-7815.	7.9	50
10	Integrated Simulation Framework for Additively Manufactured Ti-6Al-4V: Melt Pool Dynamics, Microstructure, Solid-State Phase Transformation, and Microelastic Response. Jom, 2019, 71, 3640-3655.	1.9	44
11	A phase-field model for deformation twinning. Philosophical Magazine Letters, 2011, 91, 110-121.	1.2	41
12	A phase-field model for hydride formation in polycrystalline metals: Application to Î´-hydride in zirconium alloys. Acta Materialia, 2019, 181, 262-277.	7.9	41
13	Phase-Field Modeling of Nucleation in Solid-State Phase Transformations. Jom, 2014, 66, 1520-1528.	1.9	32
14	Incorporating diffuse-interface nuclei in phase-field simulations. Scripta Materialia, 2010, 63, 8-11.	5.2	31
15	Nanointerfaceâ€Driven Reversible Hydrogen Storage in the Nanoconfined Liâ€“Nâ€“H System. Advanced Materials Interfaces, 2017, 4, 1600803.	3.7	30
16	A Mechanistic Analysis of Phase Evolution and Hydrogen Storage Behavior in Nanocrystalline Mg(BH₄)₂ within Reduced Graphene Oxide. ACS Nano, 2020, 14, 1745-1756.	14.6	29
17	Magnesium- and intermetallic alloys-based hydrides for energy storage: modelling, synthesis and properties. Progress in Energy, 2022, 4, 032007.	10.9	29
18	Microstructural impacts on ionic conductivity of oxide solid electrolytes from a combined atomistic-mesoscale approach. Npj Computational Materials, 2021, 7, .	8.7	25

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19	A Spectral Iterative Method for the Computation of Effective Properties Of Elastically Inhomogeneous Polycrystals. Communications in Computational Physics, 2012, 11, 726-738.	1.7	24
20	Elucidating the mechanism of MgB₂initial hydrogenation via a combined experimentalâ€“theoretical study. Physical Chemistry Chemical Physics, 2017, 19, 22646-22658.	2.8	23
21	Exploring the relationship between solvent-assisted ball milling, particle size, and sintering temperature in garnet-type solid electrolytes. Journal of Power Sources, 2021, 484, 229252.	7.8	23
22	Hydrogen storage in complex hydrides: past activities and new trends. Progress in Energy, 2022, 4, 032009.	10.9	23
23	The Effect of the Dehydration of MgO Films on their XPS Spectra and Electrical Properties. Journal of the Electrochemical Society, 2007, 154, J408.	2.9	22
24	Kinetic Pathways of Phase Transformations in Two-Phase Ti Alloys. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2014, 45, 3438-3445.	2.2	22
25	A phase-field model for elastically anisotropic polycrystalline binary solid solutions. Philosophical Magazine, 2013, 93, 1468-1489.	1.6	17
26	Nanoscale Mgâ€“B via Surfactant Ball Milling of MgB₂: Morphology, Composition, and Improved Hydrogen Storage Properties. Journal of Physical Chemistry C, 2020, 124, 21761-21771.	3.1	17
27	Theoretical Assessment on the Phase Transformation Kinetic Pathways of Multi-component Ti Alloys: Application to Ti-6Al-4V. Journal of Phase Equilibria and Diffusion, 2016, 37, 53-64.	1.4	16
28	Semi-Automated Creation of Density Functional Tight Binding Models through Leveraging Chebyshev Polynomial-Based Force Fields. Journal of Chemical Theory and Computation, 2021, 17, 4435-4448.	5.3	16
29	Towards understanding particle rigid-body motion during solid-state sintering. Journal of the European Ceramic Society, 2021, 41, 211-231.	5.7	16
30	Universal roles of hydrogen in electrochemical performance of graphene: high rate capacity and atomistic origins. Scientific Reports, 2015, 5, 16190.	3.3	15
31	Phase-field model of deformation twin-grain boundary interactions in hexagonal systems. Acta Materialia, 2020, 200, 821-834.	7.9	15
32	Beyond Idealized Models of Nanoscale Metal Hydrides for Hydrogen Storage. Industrial & Engineering Chemistry Research, 2020, 59, 5786-5796.	3.7	15
33	Hydriding of titanium: Recent trends and perspectives in advanced characterization and multiscale modeling. Current Opinion in Solid State and Materials Science, 2022, 26, 101020.	11.5	15
34	Phase field model of deformation twinning in tantalum: Parameterization via molecular dynamics. Scripta Materialia, 2013, 68, 451-454.	5.2	14
35	Ground-State and Thermodynamical Properties of Uranium Mononitride from Anharmonic First-Principles Theory. Applied Sciences (Switzerland), 2019, 9, 3914.	2.5	14
36	A mesoscopic digital twin that bridges length and time scales for control of additively manufactured metal microstructures. JPhys Materials, 2021, 4, 034012.	4.2	14

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37	Hydride-based thermal energy storage. Progress in Energy, 2022, 4, 032008.	10.9	14
38	Research and development of hydrogen carrier based solutions for hydrogen compression and storage. Progress in Energy, 2022, 4, 042005.	10.9	14
39	Phase-field modeling of diffusional phase behaviors of solid surfaces: A case study of phase-separating Li FePO4 electrode particles. Computational Materials Science, 2015, 108, 323-332.	3.0	11
40	Effect of medium range order on pulsed laser crystallization of amorphous germanium thin films. Applied Physics Letters, 2016, 108, 221906.	3.3	11
41	Defects, Entropy, and the Stabilization of Alternative Phase Boundary Orientations in Battery Electrode Particles. Advanced Energy Materials, 2016, 6, 1501759.	19.5	11
42	Morphologyâ€Đependent Stability of Complex Metal Hydrides and Their Intermediates Using Firstâ€Principles Calculations. ChemPhysChem, 2019, 20, 1340-1347.	2.1	11
43	Critical nuclei at hetero-phase interfaces. Acta Materialia, 2020, 200, 510-525.	7.9	11
44	Molecular dynamics studies of fundamental bulk properties of palladium hydrides for hydrogen storage. Journal of Applied Physics, 2018, 123, .	2.5	10
45	A novel liquid-mediated nucleation mechanism for explosive crystallization in amorphous germanium. Acta Materialia, 2019, 179, 190-200.	7.9	10
46	Formation of high purity uranium via laser induced thermal decomposition of uranium nitride. Materials and Design, 2020, 192, 108706.	7.0	8
47	Hydrogen Storage Performance of Preferentially Oriented Mg/rGO Hybrids. Chemistry of Materials, 2022, 34, 2963-2971.	6.7	8
48	Enhancement of effective thermal conductivity of rGO/Mg nanocomposite packed beds. International Journal of Heat and Mass Transfer, 2022, 192, 122891.	4.8	8
49	Effects of O[sub 2] Ambient on the Properties of MgO Thin Films Deposited by E-Beam Evaporation. Journal of the Electrochemical Society, 2007, 154, J352.	2.9	6
50	Understanding Charge Transfer at Mg/MgH ₂ Interfaces for Hydrogen Storage. ECS Transactions, 2017, 77, 81-90.	0.5	6
51	Chemomechanical effect of reduced graphene oxide encapsulation on hydrogen storage performance of Pd nanoparticles. Journal of Materials Chemistry A, 2021, 9, 11641-11650.	10.3	6
52	Spinodal twinning of a deformed crystal. Philosophical Magazine, 2014, 94, 888-897.	1.6	4
53	On Thermodynamic and Kinetic Mechanisms for Stabilizing Surface Solid Solutions. ACS Applied Materials & Interfaces, 2019, 11, 48487-48496.	8.0	4
54	Laser-induced thermal decomposition of uranium triiodide and ammonium uranium fluoride. Journal of Radioanalytical and Nuclear Chemistry, 2021, 329, 1427-1437.	1.5	4

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55	Understanding Hydrogenation Chemistry at MgB₂Reactive Edges fromAb InitioMolecular Dynamics. ACS Applied Materials & Interfaces, 2022, 14, 20430-20442.	8.0	4
56	An Analytical Bond Order Potential for Mgâ"H Systems. ChemPhysChem, 2019, 20, 1404-1411.	2.1	3
57	Modeling the thermodynamics of the FeTi hydrogenation under para-equilibrium: An ab-initio and experimental study. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2022, 77, 102426.	1.6	3
58	Semiempirical method for calculation of secondary electron emission coefficients of insulating materials using their spectra of x-ray photoelectron spectroscopy. Journal of Materials Research, 2007, 22, 3178-3185.	2.6	2
59	Finite-Temperature Behavior of PdHx Elastic Constants Computed by Direct Molecular Dynamics. MRS Advances, 2017, 2, 3341-3346.	0.9	2
60	Thermodynamics of Uranium Tri-Iodide from Density-Functional Theory. Applied Sciences (Switzerland), 2020, 10, 3914.	2.5	2
61	Phase-field Model for Diffusional Phase Transformations in Elastically Inhomogeneous Polycrystals. Solid State Phenomena, 0, 172-174, 1084-1089.	0.3	1
62	The effects of (Ba,Sr,Ca)CO₃ or LaB₆ addition on the x-ray photoelectron spectroscopy spectra and electrical properties of the MgO thin films in alternating current plasma display panels. Journal of Materials Research, 2008, 23, 444-451.	2.6	0