Tae Wook Heo

List of Publications by Year in Descending Order

55 papers	1,181 citations	17 h-index	33 g-index
62 ext. papers	1,534 ext. citations	6.9 avg, IF	4.67 L-index

#	Paper	IF	Citations
55	Enhancement of effective thermal conductivity of rGO/Mg nanocomposite packed beds. *International Journal of Heat and Mass Transfer*, **2022**, 192, 122891	4.9	1
54	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	1.9	0
53	A mesoscopic digital twin that bridges length and time scales for control of additively manufactured metal microstructures. *JPhys Materials*, **2021**, 4, 034012	4.2	3
52	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	6.4	5
51	Laser-induced thermal decomposition of uranium triiodide and ammonium uranium fluoride. *Journal of Radioanalytical and Nuclear Chemistry*, **2021**, 329, 1427-1437	1.5	1
50	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	8.9	12
49	Towards understanding particle rigid-body motion during solid-state sintering. *Journal of the European Ceramic Society*, **2021**, 41, 211-211	6	3
48	Chemomechanical effect of reduced graphene oxide encapsulation on hydrogen storage performance of Pd nanoparticles. *Journal of Materials Chemistry A*, **2021**, 9, 11641-11650	13	1
47	Microstructural impacts on ionic conductivity of oxide solid electrolytes from a combined atomistic-mesoscale approach. *Npj Computational Materials*, **2021**, 7,	10.9	4
46	Critical nuclei at hetero-phase interfaces. *Acta Materialia*, **2020**, 200, 510-525	8.4	5
45	Thermodynamics of Uranium Tri-Iodide from Density-Functional Theory. *Applied Sciences (Switzerland)*, **2020**, 10, 3914	2.6	2
44	Beyond Idealized Models of Nanoscale Metal Hydrides for Hydrogen Storage. *Industrial & Engineering Chemistry Research*, **2020**, 59, 5786-5796	3.9	6
43	Formation of high purity uranium via laser induced thermal decomposition of uranium nitride. *Materials and Design*, **2020**, 192, 108706	8.1	4
42	A Mechanistic Analysis of Phase Evolution and Hydrogen Storage Behavior in Nanocrystalline Mg(BH) within Reduced Graphene Oxide. *ACS Nano*, **2020**, 14, 1745-1756	16.7	12
41	Microstructural control in metal laser powder bed fusion additive manufacturing using laser beam shaping strategy. *Acta Materialia*, **2020**, 184, 284-305	8.4	79
40	Phase-field model of deformation twin-grain boundary interactions in hexagonal systems. *Acta Materialia*, **2020**, 200, 821-834	8.4	4
39	Nanoscale MgB via Surfactant Ball Milling of MgB2: Morphology, Composition, and Improved Hydrogen Storage Properties. *Journal of Physical Chemistry C*, **2020**, 124, 21761-21771	3.8	7

38	A novel liquid-mediated nucleation mechanism for explosive crystallization in amorphous germanium. *Acta Materialia*, **2019**, 179, 190-200	8.4	5
37	Morphology-Dependent Stability of Complex Metal Hydrides and Their Intermediates Using First-Principles Calculations. *ChemPhysChem*, **2019**, 20, 1340-1347	3.2	8
36	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	2.1	26
35	A phase-field model for hydride formation in polycrystalline metals: Application to δ-hydride in zirconium alloys. *Acta Materialia*, **2019**, 181, 262-277	8.4	18
34	Ground-State and Thermodynamical Properties of Uranium Mononitride from Anharmonic First-Principles Theory. *Applied Sciences (Switzerland)*, **2019**, 9, 3914	2.6	9
33	On Thermodynamic and Kinetic Mechanisms for Stabilizing Surface Solid Solutions. *ACS Applied Materials & Interfaces*, **2019**, 11, 48487-48496	9.5	2
32	An Analytical Bond Order Potential for Mg-H Systems. *ChemPhysChem*, **2019**, 20, 1404-1411	3.2	2
31	Molecular dynamics studies of fundamental bulk properties of palladium hydrides for hydrogen storage. *Journal of Applied Physics*, **2018**, 123, 225105	2.5	4
30	Nanostructured Metal Hydrides for Hydrogen Storage. *Chemical Reviews*, **2018**, 118, 10775-10839	68.1	256
29	Nanointerface-Driven Reversible Hydrogen Storage in the Nanoconfined Li□□H System. *Advanced Materials Interfaces*, **2017**, 4, 1600803	4.6	20
28	Understanding Charge Transfer at Mg/MgH2 Interfaces for Hydrogen Storage. *ECS Transactions*, **2017**, 77, 81-90	1	4
27	Understanding Ionic Conductivity Trends in Polyborane Solid Electrolytes from Ab Initio Molecular Dynamics. *ACS Energy Letters*, **2017**, 2, 250-255	20.1	64
26	Structural, Chemical, and Dynamical Frustration: Origins of Superionic Conductivity in closo-Borate Solid Electrolytes. *Chemistry of Materials*, **2017**, 29, 9142-9153	9.6	103
25	Hierarchically Controlled Inside-Out Doping of Mg Nanocomposites for Moderate Temperature Hydrogen Storage. *Advanced Functional Materials*, **2017**, 27, 1704316	15.6	49
24	Finite-Temperature Behavior of PdHx Elastic Constants Computed by Direct Molecular Dynamics. *MRS Advances*, **2017**, 2, 3341-3346	0.7	2
23	Elucidating the mechanism of MgB initial hydrogenation via a combined experimental-theoretical study. *Physical Chemistry Chemical Physics*, **2017**, 19, 22646-22658	3.6	16
22	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	14
21	Effect of medium range order on pulsed laser crystallization of amorphous germanium thin films. *Applied Physics Letters*, **2016**, 108, 221906	3.4	9

20	Defects, Entropy, and the Stabilization of Alternative Phase Boundary Orientations in Battery Electrode Particles. *Advanced Energy Materials*, **2016**, 6, 1501759	21.8	11
19	Phase-field modeling of diffusional phase behaviors of solid surfaces: A case study of phase-separating LiXFePO4 electrode particles. *Computational Materials Science*, **2015**, 108, 323-332	3.2	9
18	Universal roles of hydrogen in electrochemical performance of graphene: high rate capacity and atomistic origins. *Scientific Reports*, **2015**, 5, 16190	4.9	13
17	Kinetic Pathways of Phase Transformations in Two-Phase Ti Alloys. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2014**, 45, 3438-3445	2.3	21
16	Toward an integrated computational system for describing the additive manufacturing process for metallic materials. *Additive Manufacturing*, **2014**, 1-4, 52-63	6.1	54
15	Phase-Field Modeling of Nucleation in Solid-State Phase Transformations. *Jom*, **2014**, 66, 1520-1528	2.1	28
14	Phase-field modeling of displacive phase transformations in elastically anisotropic and inhomogeneous polycrystals. *Acta Materialia*, **2014**, 76, 68-81	8.4	49
13	Spinodal twinning of a deformed crystal. *Philosophical Magazine*, **2014**, 94, 888-897	1.6	4
12	Phase field model of deformation twinning in tantalum: Parameterization via molecular dynamics. *Scripta Materialia*, **2013**, 68, 451-454	5.6	14
11	A phase-field model for elastically anisotropic polycrystalline binary solid solutions. *Philosophical Magazine*, **2013**, 93, 1468-1489	1.6	14
10	A Spectral Iterative Method for the Computation of Effective Properties Of Elastically Inhomogeneous Polycrystals. *Communications in Computational Physics*, **2012**, 11, 726-738	2.4	17
9	A phase field study of strain energy effects on solute–grain boundary interactions. *Acta Materialia*, **2011**, 59, 7800-7815	8.4	45
8	A phase-field model for deformation twinning. *Philosophical Magazine Letters*, **2011**, 91, 110-121	1	36
7	A phase-field model of stress effect on grain boundary migration. *Modelling and Simulation in Materials Science and Engineering*, **2011**, 19, 035002	2	44
6	Phase-field Model for Diffusional Phase Transformations in Elastically Inhomogeneous Polycrystals. *Solid State Phenomena*, **2011**, 172-174, 1084-1089	0.4	1
5	Incorporating diffuse-interface nuclei in phase-field simulations. *Scripta Materialia*, **2010**, 63, 8-11	5.6	30
4	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	2.5	
3	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	2.5	2

2	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	3.9	5
1	The Effect of the Dehydration of MgO Films on their XPS Spectra and Electrical Properties. *Journal of the Electrochemical Society*, **2007**, 154, J408	3.9	16