

# Young-Su Lee

## List of Publications by Year in descending order

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96  
papers

7,802  
citations

136740

32  
h-index

49773

87  
g-index

100  
all docs

100  
docs citations

100  
times ranked

7575  
citing authors

#	ARTICLE	IF	CITATIONS
1	wannier90: A tool for obtaining maximally-localised Wannier functions. Computer Physics Communications, 2008, 178, 685-699.	3.0	2,947
2	An updated version of wannier90: A tool for obtaining maximally-localised Wannier functions. Computer Physics Communications, 2014, 185, 2309-2310.	3.0	1,561
3	Complex hydrides for hydrogen storage – new perspectives. Materials Today, 2014, 17, 122-128.	8.3	408
4	Band Structure and Quantum Conductance of Nanostructures from Maximally Localized Wannier Functions: The Case of Functionalized Carbon Nanotubes. Physical Review Letters, 2005, 95, 076804.	2.9	187
5	Boron–nitrogen based hydrides and reactive composites for hydrogen storage. Materials Today, 2014, 17, 129-135.	8.3	165
6	Cycloaddition Functionalizations to Preserve or Control the Conductance of Carbon Nanotubes. Physical Review Letters, 2006, 97, 116801.	2.9	133
7	LiCe(BH <sub>4</sub> ) <sub>3</sub> Cl, a New Lithium-Ion Conductor and Hydrogen Storage Material with Isolated Tetranuclear Anionic Clusters. Chemistry of Materials, 2012, 24, 1654-1663.	3.2	128
8	Decomposition Reactions and Reversibility of the LiBH <sub>4</sub> –Ca(BH <sub>4</sub> ) <sub>2</sub> Composite. Journal of Physical Chemistry C, 2009, 113, 15080-15086.	1.5	105
9	Spin Channels in Functionalized Graphene Nanoribbons. Nano Letters, 2009, 9, 3425-3429.	4.5	103
10	Reversible Hydrogen Storage in LiBH <sub>4</sub> –MH <sub>2</sub> (M = Ce, Ca) Composites. Journal of Physical Chemistry C, 2008, 112, 9520-9524.	1.5	95
11	Identification of the Dehydrogenated Product of Ca(BH <sub>4</sub> ) <sub>2</sub> . Journal of Physical Chemistry C, 2009, 113, 5865-5871.	1.5	82
12	Effect of Hydrogen Back Pressure on Dehydrogenation Behavior of LiBH <sub>4</sub> -Based Reactive Hydride Composites. Journal of Physical Chemistry Letters, 2010, 1, 59-63.	2.1	76
13	Interface-enhanced Li ion conduction in a LiBH <sub>4</sub> –SiO <sub>2</sub> solid electrolyte. Physical Chemistry Chemical Physics, 2016, 18, 22540-22547.	1.3	72
14	The mechanism of Mg <sup>2+</sup> conduction in ammine magnesium borohydride promoted by a neutral molecule. Physical Chemistry Chemical Physics, 2020, 22, 9204-9209.	1.3	70
15	Ammonia-assisted fast Li-ion conductivity in a new hemiammine lithium borohydride, LiBH <sub>4</sub> ·1/2NH <sub>3</sub> . Chemical Communications, 2020, 56, 3971-3974.	2.2	60
16	Enhanced Li Ion Conductivity in LiBH <sub>4</sub> –Al <sub>2</sub> O <sub>3</sub> Mixture via Interface Engineering. Journal of Physical Chemistry C, 2017, 121, 26209-26215.	1.5	57
17	Enhanced Desorption and Absorption Properties of Eutectic LiBH <sub>4</sub> –Ca(BH <sub>4</sub> ) <sub>2</sub> Infiltrated into Mesoporous Carbon. Journal of Physical Chemistry C, 2011, 115, 20027-20035.	1.5	48
18	Hydrogen-induced interactions in vanadium from first-principles calculations. Physical Review B, 2011, 83, .	1.1	45

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19	Structural and magnetocaloric properties of novel gadolinium borohydrides. <i>Journal of Alloys and Compounds</i> , 2016, 664, 378-384.	2.8	45
20	Metal halide doped metal borohydrides for hydrogen storage: The case of $\text{Ca}(\text{BH}_4)_2 \cdot \text{CaX}_2$ (X=F, Cl) mixture. <i>Journal of Alloys and Compounds</i> , 2010, 506, 721-727.	2.8	44
21	Numerical simulation of long-term precipitate evolution in austenitic heat-resistant steels. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2010, 34, 105-112.	0.7	44
22	Synthesis and Structural Investigation of $\text{Zr}(\text{BH}_4)_4$ . <i>Journal of Physical Chemistry C</i> , 2012, 116, 20239-20245.	1.5	43
23	Synthesis, Crystal Structure, Thermal Decomposition, and $^{11}\text{B}$ MAS NMR Characterization of $\text{Mg}(\text{BH}_4)_2(\text{NH}_3\text{BH}_3)_2$ . <i>Journal of Physical Chemistry C</i> , 2014, 118, 12141-12153.	1.5	41
24	Trends in Syntheses, Structures, and Properties for Three Series of Ammine Rare-Earth Metal Borohydrides, $\text{M}(\text{BH}_4)_3 \cdot \text{nNH}_3$ (M = Y, Gd, and Dy). <i>Inorganic Chemistry</i> , 2015, 54, 7402-7414.	1.9	41
25	Enhancing the Hydrogen Storage Properties of $\text{A}_x\text{B}_y$ Intermetallic Compounds by Partial Substitution: A Short Review. <i>Hydrogen</i> , 2020, 1, 38-63.	1.7	38
26	Investigation of the Dehydrogenation Reaction Pathway of $\text{Ca}(\text{BH}_4)_2$ and Reversibility of Intermediate Phases. <i>Journal of Physical Chemistry C</i> , 2012, 116, 4330-4334.	1.5	37
27	Solid state synthesis, structural characterization and ionic conductivity of bimetallic alkali-metal yttrium borohydrides $\text{MY}(\text{BH}_4)_4$ (M = Li and Na). <i>Journal of Materials Chemistry A</i> , 2016, 4, 8793-8802.	5.2	37
28	Crystal structure and phonon instability of high-temperature $\text{Ca}(\text{BH}_4)_2$ . <i>Physical Review B</i> , 2009, 79, .	1.1	36
29	Rehydrogenation and cycle studies of $\text{LiBH}_4 \cdot \text{CaH}_2$ composite. <i>International Journal of Hydrogen Energy</i> , 2010, 35, 6578-6582.	3.8	35
30	Dehydrogenation behavior of $\text{LiBH}_4/\text{CaH}_2$ composite with $\text{NbF}_5$ . <i>Scripta Materialia</i> , 2008, 59, 1251-1254.	2.6	33
31	A mixed-cation mixed-anion borohydride $\text{NaY}(\text{BH}_4)_2\text{Cl}_2$ . <i>International Journal of Hydrogen Energy</i> , 2012, 37, 8428-8438.	3.8	33
32	Is $\text{Y}_2(\text{B}_{12}\text{H}_{12})_3$ the main intermediate in the decomposition process of $\text{Y}(\text{BH}_4)_3$ ? <i>Chemical Communications</i> , 2013, 49, 5234.	2.2	33
33	Polymorphism and Thermodynamics of $\text{Y}(\text{BH}_4)_3$ from First Principles. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12833-12837.	1.5	32
34	Metastable hexagonal close-packed palladium hydride in liquid cell TEM. <i>Nature</i> , 2022, 603, 631-636.	18.7	31
35	Kinetics and thermodynamics of near eutectic Mg-Mg <sub>2</sub> Ni composites produced by casting process. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 29009-29022.	3.8	28
36	Role of alloying elements in vanadium-based binary alloy membranes for hydrogen separation. <i>Journal of Membrane Science</i> , 2012, 423-424, 332-341.	4.1	26

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37	Metallic and complex hydride-based electrochemical storage of energy. <i>Progress in Energy</i> , 2022, 4, 032001.	4.6	26
38	Direct measurement of hydrogen diffusivity through Pd-coated Ni-based amorphous metallic membranes. <i>Journal of Membrane Science</i> , 2013, 436, 195-201.	4.1	25
39	Enhanced high temperature hydrogen permeation characteristics of $\text{Ni}$ alloy membranes containing a trace amount of yttrium. <i>Scripta Materialia</i> , 2016, 116, 122-126.	2.6	25
40	Microscopic Origin of Universal Quasilinear Band Structures of Transparent Conducting Oxides. <i>Physical Review Letters</i> , 2012, 108, 196404.	2.9	24
41	Hydrogen Back-Pressure Effects on the Dehydrogenation Reactions of $\text{Ca}(\text{BH}_4)_2$ . <i>Journal of Physical Chemistry C</i> , 2012, 116, 25715-25720.	1.5	24
42	Prediction of hydrogen permeability in $\text{Al}$ and $\text{Ni}$ alloys. <i>Journal of Membrane Science</i> , 2013, 430, 234-241.	4.1	24
43	Ammine Calcium and Strontium Borohydrides: Syntheses, Structures, and Properties. <i>ChemSusChem</i> , 2015, 8, 3472-3482.	3.6	24
44	In Situ NMR Study on the Interaction between $\text{LiBH}_4$ and $\text{Ca}(\text{BH}_4)_2$ and Mesoporous Scaffolds. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2922-2927.	2.1	23
45	Tailoring the equilibrium hydrogen pressure of TiFe via vanadium substitution. <i>Journal of Alloys and Compounds</i> , 2021, 854, 157263.	2.8	23
46	Effect of Cr addition on room temperature hydrogenation of TiFe alloys. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 19478-19485.	3.8	23
47	Hydrogen storage in complex hydrides: past activities and new trends. <i>Progress in Energy</i> , 2022, 4, 032009.	4.6	23
48	Cycloadditions to Control Bond Breaking in Naphthalenes, Fullerenes, and Carbon Nanotubes: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2008, 112, 4480-4485.	1.5	22
49	Synthesis of $\text{Mg}_2\text{FeH}_6$ by hydrogenation of Mg/Fe powder mixture prepared by cold roll milling in air: Effects of microstructure and oxygen distribution. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 16758-16765.	3.8	22
50	Hydrogen storage behavior and microstructural feature of a TiFe-ZrCr <sub>2</sub> alloy. <i>Journal of Alloys and Compounds</i> , 2021, 853, 157099.	2.8	22
51	Low temperature formation of $\text{Mg}_2\text{FeH}_6$ by hydrogenation of ball-milled nano-crystalline powder mixture of Mg and Fe. <i>Materials and Design</i> , 2017, 135, 239-245.	3.3	21
52	Controlling the Dehydrogenation Reaction toward Reversibility of the $\text{LiBH}_4$ - $\text{Ca}(\text{BH}_4)_2$ Eutectic System. <i>Journal of Physical Chemistry C</i> , 2013, 117, 8878-8886.	1.5	20
53	Lithium Ion Disorder and Conduction Mechanism in $\text{LiCe}(\text{BH}_4)_3\text{Cl}$ . <i>Journal of Physical Chemistry C</i> , 2016, 120, 19035-19042.	1.5	20
54	Activation of Ti-Fe-Cr alloys containing identical AB <sub>2</sub> fractions. <i>Journal of Alloys and Compounds</i> , 2021, 864, 158876.	2.8	20

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55	On the Formation and the Structure of the First Bimetallic Borohydride Borate, $\text{LiCa}_3(\text{BH}_4)_4(\text{BO}_3)_2$ . Journal of Physical Chemistry C, 2011, 115, 10298-10304.	1.5	19
56	Thermodynamics of the dehydrogenation of the $\text{LiBH}_4\text{-YH}_3$ composite: Experimental and theoretical studies. Journal of Alloys and Compounds, 2012, 510, L9-L12.	2.8	19
57	Long term high temperature oxidation characteristics of La and Cu alloyed ferritic stainless steels for solid oxide fuel cell interconnects. Journal of Power Sources, 2016, 327, 104-118.	4.0	19
58	Ammine Lanthanum and Cerium Borohydrides, $\text{M}(\text{BH}_4)_3 \cdot \text{nNH}_3$ ; Trends in Synthesis, Structures, and Thermal Properties. Inorganic Chemistry, 2020, 59, 7768-7778.	1.9	19
59	Mitigation of degradation in the dehydrogenation behavior of air-exposed $\text{MgH}_2$ catalyzed with $\text{NbF}_5$ . Journal of Alloys and Compounds, 2013, 575, 393-398.	2.8	18
60	Thermal properties of $\text{Y}(\text{BH}_4)_3$ synthesized via two different methods. International Journal of Hydrogen Energy, 2013, 38, 9263-9270.	3.8	17
61	Si/iron silicide nanocomposite anodes with furfuryl-alcohol-derived carbon coating for Li-ion batteries. Journal of Materials Science, 2017, 52, 5027-5037.	1.7	17
62	Hydrogenation reaction of $\text{CaH}_2\text{-CaB}_6\text{-Mg}$ mixture. Journal of Alloys and Compounds, 2010, 492, 597-600.	2.8	16
63	Structural Diversity and Trends in Properties of an Array of Hydrogen-Rich Ammonium Metal Borohydrides. Inorganic Chemistry, 2020, 59, 12733-12747.	1.9	16
64	Understanding first cycle hydrogenation properties of $\text{Ti-Fe-Zr}$ ternary alloys. International Journal of Hydrogen Energy, 2021, 46, 4241-4251.	3.8	15
65	Mechanism for Z-phase formation in 11CrMoVNbN martensitic heat-resistant steel. Materials Characterization, 2017, 129, 40-45.	1.9	14
66	Probing molecular dynamics of metal borohydrides on the surface of mesoporous scaffolds by multinuclear high resolution solid state NMR. Journal of Alloys and Compounds, 2015, 645, S316-S319.	2.8	13
67	The role of Fe particle size and oxide distribution on the hydrogenation properties of ball-milled nano-crystalline powder mixtures of Fe and Mg. Journal of Alloys and Compounds, 2019, 806, 1039-1046.	2.8	13
68	Discovery of Fluidic $\text{LiBH}_4$ on Scaffold Surfaces and Its Application for Fast Co-confinement of $\text{LiBH}_4\text{-Ca}(\text{BH}_4)_2$ into Mesopores. Journal of Physical Chemistry C, 2015, 119, 9025-9035.	1.5	12
69	Fast Lithium Ion Migration in Room Temperature $\text{LiBH}_4$ . Journal of Physical Chemistry C, 2017, 121, 17773-17779.	1.5	12
70	Mechanochemical synthesis of $\text{Ce}_3\text{Al}_{11}$ powder and its catalytic effect on the hydrogen sorption properties of $\text{NaAlH}_4$ . Journal of Alloys and Compounds, 2019, 784, 313-318.	2.8	12
71	A finite outlet volume correction to the time lag method: The case of hydrogen permeation through V-alloy and Pd membranes. Journal of Membrane Science, 2019, 585, 253-259.	4.1	11
72	Atomistic simulation of hydrogen diffusion at tilt grain boundaries in vanadium. Metals and Materials International, 2013, 19, 1221-1225.	1.8	10

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73	Crystal Structures and Energy Storage Properties of Ammine Sodium Decahydro-closo-decaboranes ( $\text{Na}_2\text{B}_{10}\text{H}_{10}\text{A}^n\text{NH}_3$ , $n = 1, 2$ ). <i>Journal of Physical Chemistry C</i> , 2019, 123, 20160-20166.	1.5	10
74	Oxidation behavior and area specific resistance of La, Cu and B alloyed Fe-22Cr ferritic steels for solid oxide fuel cell interconnects. <i>Journal of Power Sources</i> , 2017, 369, 13-26.	4.0	9
75	A modified embedded-atom method interatomic potential for the V-H system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2011, 35, 302-307.	0.7	8
76	First-principles study on the thermal expansion of Ni-X binary alloys based on the quasi-harmonic Debye model. <i>Metals and Materials International</i> , 2016, 22, 1065-1072.	1.8	8
77	Hydrogen occupation in $\text{Ti}_4\text{M}_2\text{O}$ compounds ( $M = \text{Fe, Co, Ni, Cu}$ , and $y = 0, 1$ ) and their hydrogen storage characteristics. <i>Journal of Alloys and Compounds</i> , 2022, 891, 162050.	2.8	8
78	Surface reaction kinetics in oxygen nonstoichiometry re-equilibration of $\text{BaTiO}_3$ . <i>Solid State Ionics</i> , 2003, 160, 381-387.	1.3	7
79	Mechanochemical synthesis of $\text{CeB}_6$ nanopowder. <i>Ceramics International</i> , 2019, 45, 19442-19446.	2.3	7
80	Mechanical property change and precipitate evolution during long-term aging of 1.25Cr-0.5Mo steel. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2020, 789, 139663.	2.6	7
81	Ammonium-Ammonia Complexes, $\text{N}_2\text{H}_7^+$ , in Ammonium closo-Borate Amines: Synthesis, Structure, and Properties. <i>Inorganic Chemistry</i> , 2020, 59, 11449-11458.	1.9	6
82	Design of V-Substituted TiFe-Based Alloy for Target Pressure Range and Easy Activation. <i>Materials</i> , 2021, 14, 4829.	1.3	6
83	Current-voltage characteristic of $\text{BaTiO}_3$ in its mixed n/p regime under oxygen potential gradients. <i>Solid State Ionics</i> , 2002, 150, 373-382.	1.3	5
84	Predictions on atomic structures of $\text{Ti}_{1-x}\text{MoxC}$ using combined approach of first-principles calculation and the cluster expansion method. <i>Metals and Materials International</i> , 2009, 15, 797-801.	1.8	5
85	Prediction of elastic properties of precipitation-hardened aluminum cast alloys. <i>Computational Materials Science</i> , 2012, 51, 365-371.	1.4	5
86	Disorder induced polymorphic transitions in the high hydrogen density compound $\text{Sr}(\text{BH}_4)_2(\text{NH}_3)_3(\text{BH}_3)_2$ . <i>Dalton Transactions</i> , 2018, 47, 16737-16746.	1.6	5
87	Synthesis and crystal structures of decahydro-closo-decaborates of the divalent cations of strontium and manganese. <i>Journal of Solid State Chemistry</i> , 2021, 298, 122133.	1.4	5
88	Identifying the nature of interaction between $\text{LiBH}_4$ and two-dimensional substrates: DFT study with van der Waals correction. <i>Journal of Alloys and Compounds</i> , 2014, 587, 428-436.	2.8	4
89	Effect of thermodynamic properties on the infrared radiation behavior of Ti-based solid solutions. <i>Journal of Alloys and Compounds</i> , 2016, 656, 753-757.	2.8	4
90	EBSD microstructural analysis of AB-type TiFe hydrogen storage alloys. <i>Materials Characterization</i> , 2021, 178, 111276.	1.9	3

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91	Prediction of Pressure-Composition-Temperature Curves of AB <sub>2</sub> -Type Hydrogen Storage Alloys by Machine Learning. <i>Metals and Materials International</i> , 2023, 29, 861-869.	1.8	3
92	Investigation of the surface chemical and electronic states of pyridine-capped CdSe nanocrystal films after plasma treatments using H <sub>2</sub> , O <sub>2</sub> , and Ar gases. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2010, 28, 559-563.	0.9	2
93	Effect of Thermal Charging of Hydrogen on the Microstructure of Metastable Austenitic Stainless Steel. <i>Steel Research International</i> , 2017, 88, 1600063.	1.0	2
94	Microstructural Analysis of Dehydrogenation Products of the Ca(BH <sub>4</sub> ) <sub>2</sub> •MgH <sub>2</sub> Composite. <i>Microscopy and Microanalysis</i> , 2013, 19, 149-151.	0.2	1
95	Thermodynamics and sorption reaction of some light metal borohydrides for reversible hydrogen storage. , 2010, , .		0
96	Effect of Ti Addition on Yield Strength of Low-Mo Fire-Resistant Steel at Elevated Temperatures. <i>Steel Research International</i> , 2023, 94, .	1.0	0