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Research Topics

First-principles simulation
Solid-state hydrogen storage materials
Hydrogen separation membranes
Ion conduction in complex hydrides

Professional Experience

Mar 2017 – Principal Research Scientist
Oct 2007 – Feb 2017 Senior Research Scientist
Korea Institute of Science and Technology, South Korea
Aug 2006 – Aug 2007 Postdoctoral Associate
Prof. N. Marzari, Materials Science and Engineering,
Massachusetts Institute of Technology, USA

Education

Sep 2001 – Jul 2006 Ph.D., Materials Science and Engineering,
Massachusetts Institute of Technology, USA
Thesis advisor: Prof. N. Marzari
Thesis: *Electronic Structure and Quantum Conductance of Nanostructures*
Mar 1999 – Feb 2001 M.S., Materials Science and Engineering, Seoul National University, South Korea
Thesis advisor: Prof. H.-I. Yoo
Thesis: *Current-Voltage Characteristic of $BaTiO_{3-\delta}$ in an Oxygen Potential Gradient*
Mar 1995 – Feb 1999 B.S., Materials Science and Engineering, Seoul National University, South Korea

Publications, International Journal

70. J. Choi, T. Ha, J. Park, **Y.-S. Lee**, H. N. Han, J. Lee, J.-H. Shim, “Mechanochemical synthesis of Ce_3Al_{11} powder and its catalytic effect on hydrogen sorption properties of $NaAlH_4$,” *J. Alloys. Compd.* **784**, 313-318 (2019).
69. M. Jørgensen, **Y.-S. Lee**, M. Bjerring, L. H. Jepsen, Ü. Akbey, Y. W. Cho, T. R. Jensen, “Disorder Induced Polymorphic Transitions in the High Hydrogen Density Compound $Sr(BH_4)_2(NH_3BH_3)_2$,” *Dalton Trans.* **47**, 16737-16746 (2018).
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65. S. Swaminathan, Y. S. Ko, **Y.-S. Lee**, D.-I. Kim, “Oxidation behavior and area specific resistance of La, Cu and B alloyed Fe-22Cr ferritic steels for solid oxide fuel cell interconnects,” *J. Power Sources* **369**, 13-26 (2017).
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63. **Y.-S. Lee** and Y. W. Cho, “Fast Lithium Ion Migration in Room Temperature $LiBH_4$,” *J. Phys. Chem. C* **121**, 17773-17779 (2017).
62. M.-Y. Kim, S.-M. Hong, K.-H. Lee, W.-S. Jung, Y.-S. Lee, Y.-K. Lee, J.-H. Shim, “Mechanism for Z-phase formation in 11CrMoVNbN martensitic heat resistant Steel,” *Mater. Charact.* **129**, 40-45 (2017).
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59. Y. Shin, W.-S. Jung, **Y.-S. Lee**, “First-principles Study on the Thermal Expansion of Ni-X Binary Alloys Based on the Quasi-Harmonic Debye Model,” *Met. Mater. Int.* **22**, 1065-1072 (2016).

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 25. J.-Y. Suh, **Y.-S. Lee**, J.-H. Shim, H. M. Park, "Prediction of elastic properties of precipitation-hardened aluminum cast alloys," *Computational Materials Science* **51**, 365-371 (2012).
 24. H.-S. Lee, **Y.-S. Lee**, J.-Y. Suh, M. Kim, J.-S. Yu, and Y. W. Cho, "Enhanced Desorption and Absorption Properties of Eutectic $\text{LiBH}_4\text{-Ca}(\text{BH}_4)_2$ Infiltrated into Mesoporous Carbon," *J. Phys. Chem. C* **115**, 20027-20035 (2011).
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19. **Y.-S. Lee**, J.-H. Shim, and Y. W. Cho, “Polymorphism and Thermodynamics of $\text{Y}(\text{BH}_4)_3$ from First Principles,” *J. Phys. Chem. C* **114**, 12833-12837 (2010).
 18. J.-H. Lim, **J.-H. Shim**, **Y.-S. Lee**, J.-Y. Suh, Y. W. Cho, and J. Lee, “Rehydrogenation and cycle studies of $\text{LiBH}_4\text{-CaH}_2$ composite,” *Int. J. Hydrogen Energy* **35**, 6578-6582 (2010).
 17. S.-J. Wang, H. Kim, **H.-H. Park**, **Y.-S. Lee**, H. Jeon, and H. J. Chang, “Investigation of the surface chemical and electronic states of pyridine-capped CdSe nanocrystal films after plasma treatments using H_2 , O_2 , and Ar gases,” *J. Vac. Sci. Technol. A* **28**, 559-563 (2010).
 16. **J.-H. Shim**, E. Kozeschnik, W.-S. Jung, S.-C. Lee, D.-I. Kim, J.-Y. Suh, **Y.-S. Lee**, Y. W. Cho, “Numerical simulation of long-term precipitate evolution in austenitic heat-resistant steels,” *CALPHAD*. **34**, 105-112 (2010).
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 6. **Y.-S. Lee** and N. Marzari, “Cycloadditions to Control Bond Breaking in Naphthalenes, Fullerenes, and Carbon Nanotubes: A First-Principles Study,” *J. Phys. Chem. C* **112**, 4480-4485 (2008).

5. A. A. Mostofi, J. Yates, **Y.-S. Lee**, I. Souza, D. Vanderbilt, and N. Marzari, “wannier90: A tool for obtaining maximally-localised Wannier functions,” *Comput. Phys. Commun.* **178**, 685-699 (2008)
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Publications, Domestic Journal

1. K.T. Kang, K.R. Han, S.W. Nam, C.S. Kim, **Y.-S. Lee**, and H.-I. Yoo, “Preparation and properties of zirconia-based electrolytes form m-zirconia and YAG sol,” *Journal of the Korean Ceramic Society*, **38** 834 (2001).