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Employment

Oct 2007 –	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

Selected Publications

14. S. H. Hwang, **Y.-S. Lee**, and Y. W. Cho, "Identifying the nature of interaction between $LiBH_4$ and two-dimensional substrates: DFT study with van der Waals correction," *J. Alloys. Compd.* **587**, 428-436 (2014).
13. K. Park, H.-S. Lee, A. Remhof, **Y.-S. Lee**, Y. Yan, M.-Y. Kim, S. J. Kim, A. Züttel, and Y. W. Cho, "Thermal properties of $Y(BH_4)_3$ synthesized via two different methods," *Int. J. Hydrogen Energy* **38**, 9263-9270 (2013).

12. **Y.-S. Lee**, C. Ouyang, J.-Y. Suh, E. Fleury, Y. W. Cho, and J.-H. Shim, "Role of alloying elements in vanadium-based binary alloy membranes for hydrogen separations," *J. Membr Sci.* **423-424**, 332-341 (2012).

11. H.-S. Lee, S.-J. Hwang, H. K. Kim, **Y.-S. Lee**, J. Park, J.-S. Yu, and Y. W. Cho, "In Situ NMR Study on the Interaction between $LiBH_4$–$Ca(BH_4)_2$ and Mesoporous Scaffolds," *J. Phys. Chem. Lett.* **3**, 2922-2927 (2012).

10. 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 $LiBH_4$-$Ca(BH_4)_2$ Infiltrated into Mesoporous Carbon," *J. Phys. Chem. C* **115**, 20027-20035 (2011).

9. **Y.-S. Lee**, Y. Filinchuk, H.-S. Lee, J.-Y. Suh, J. W. Kim, J.-S. Yu, and Y. W. Cho, "On the formation and the structure of the first bimetallic borohydride borate, $LiCa_3(BH_4)(BO_3)_2$," *J. Phys. Chem. C* **115**, 10298-10304 (2011).

8. C. Ouyang and **Y.-S. Lee**, "Hydrogen-induced interactions in vanadium from first-principles calculations," *Phys. Rev. B* **83**, 045111 (2011).

7. **Y.-S. Lee**, J.-H. Shim, and Y. W. Cho, "Polymorphism and Thermodynamics of $Y(BH_4)_3$ from First Principles," *J. Phys. Chem. C* **114**, 12833-12837 (2010).

6. J. Y. Lee, D. Ravnsbæk, **Y.-S. Lee**, Y. Kim, Y. Cerenius, J.-H. Shim, T. R. Jensen, N. H. Hur, and Y. W. Cho, "Decomposition reactions and reversibility of the $LiBH_4$-$Ca(BH_4)_2$ composite," *J. Phys. Chem. C* **113**, 15080-15086 (2009).

5. **Y.-S. Lee**, Y. Kim, Y. W. Cho, D. Shapiro, C. Wolverton, and V. Ozolins, "Crystal structure and phonon instability of high temperature β-$Ca(BH_4)_2$," *Phys. Rev. B* **79**, 104107 (2009).

4. **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).

3. **Y.-S. Lee** and N. Marzari, "Cycloaddition functionalizations to preserve or control the conductance of carbon nanotubes," *Phys. Rev. Lett.*, **97**, 116801 (2006).

2. **Y.-S. Lee**, M.B. Nardelli, and N. Marzari, "Band structure and quantum transport of nanostructures from maximally localized Wannier functions: the case of functionalized carbon nanotubes," *Phys. Rev. Lett.*, **95**, 076804 (2005).

1. **Y.-S. Lee** and H.-I. Yoo, "Current-voltage characteristic of $BaTiO_{3-\delta}$ in its mixed n/p regime under oxygen potential gradients," *Solid State Ionics*, **150**, 373-382 (2002).