

# Yongjin Shin

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## EDUCATION

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2015 – 2020 Ph.D., Materials Science and Engineering, **Northwestern University**, IL, U.S.A.

2009 – 2014 B.S., Materials Science and Engineering, **Korea University**, Seoul, Korea

## RESEARCH EXPERIENCE

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Nov 2021 – Present **Postdoctoral Researcher**, University of Chicago, Chicago, IL, U.S.A.  
Advisor: Prof. Giulia Galli

- Explored quantum materials for neuromorphic computing devices by using first-principles calculations
- Discovered hidden perovskite phases responsible for high threshold voltage in phase transitions
- Established design principles of novel ferroelectricity in oxygen-deficient perovskites

Sep 2020 – Sep 2021 **Postdoctoral Researcher**, University of California, Santa Barbara, CA, U.S.A.  
Advisor: Prof. Chris G. Van de Walle

- Investigated a potential origin of charge trapping in a tunneling devices developed by SAMSUNG Inc.
- Formulated a quantitative modeling of capture time constant mediated by quantum tunneling, which explains experimental noise in MOSFET devices occurred by defects in SiO<sub>2</sub>
- Utilized density functional theory (DFT) to disentangle electron-phonon interaction near defects

Sep 2015 – Aug 2020 **Research Assistant**, Northwestern University, IL, U.S.A.  
Advisor: Prof. James M. Rondinelli

- Implemented a structure generation algorithm for perovskite structure with ordered oxygen vacancies
- Formulated a quantitative theory of stability in perovskite-derived structure, such as brownmillerite (A<sub>2</sub>B<sub>2</sub>O<sub>5</sub>), Ruddlesden-Popper phase (A<sub>2</sub>BO<sub>4</sub>), based on DFT
- Identified novel phenomena in complex oxides such as magnetic transitions, magnetoelastic coupling, and two-dimensional electron gas

Jul 2014 – Sep 2015 **Researcher**, Korea Institute of Science and Technology, Seoul, Korea  
Advisor: Dr. Young-Su Lee

- Designed Ni-based super alloy of advanced properties such as high thermal stability and low thermal expansion coefficient via introducing additives like Co, Ta, W, and Re
- Developed in-house numerical code to calculate thermal expansion based on parameters obtained from DFT calculations.

Jul 2013 – Dec 2013 **Intern Engineer**, General Electric Ultrasound Korea, Sunnam, Korea

- Developed an ultrasound machine for medical use; collected pulse wave data using a piezoelectric probe
- Renovated the measurement process based on big data of pulse signal; examined the correlation among input parameters affecting acoustic properties

Oct 2011 – Aug 2012 **Intern Student Researcher**, Ian Wark Research Institute, Australia

- Inspected the kinetics of a hydrophobic drug delivery in Polyelectrolyte Multilayers (PEM)
- Evaluated major mechanism of releasing kinetics by comparing *in-situ* and *ex-situ* spectroscopy: UV-vis, ATR-FTIR, and QCM-D

Jul 2011 **Summer Research Program**, Korea Advanced Institute of Science and Technology, Korea

- Investigated thermal stability of silver nanowire: studied energetics between wire with pentagonal cross-section and wire with FCC structure with DFT

## HONORS AND AWARDS

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2020	<i>Ovshinsky Student Travel Awards</i> by American Physical Society
2019	<i>Graduate Scholarship</i> by Korean-American Scientists and Engineers Association
2015	<i>The Korean Government Scholarship Program for Study Overseas</i>
2013	<i>Gold Medal</i> in Engineering Career Portfolio Exposition Accreditation Board for Engineering Education of Korea (ABEEK)
2011	<i>Best Presentation</i> in summer research program, KAIST
2011	<i>Venture Internship Program Scholarships</i> , Korean government
Undergrad	<i>Admission Scholarship for excellent grade (4yrs)</i> , Korea University
Undergrad	<i>National Science &amp; Technology Scholarship (4yrs)</i> , Korean government
Undergrad	<i>Semester High Honors</i> at Korea University in 2009 (Spring, Fall), 2010 (Fall), 2012 (Fall), and 2013 (Spring)

## PUBLICATIONS

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1. **Y. Shin**, M. Turiansky, B. Lee, and C. G. Van de Walle, "Modeling carrier trapping at semiconductor/dielectric interfaces based on first-principles calculations of nonradiative capture" *in writing*
2. **Y. Shin**, K. R. Poeppelmeier, and J. M. Rondinelli, "Informatics-based learning of oxygen vacancy ordering principles in oxygen-deficient perovskites" *in writing*
3. Z. Yan, K. G. Reynolds, Rui Sun, **Y. Shin**, A. E. Thorarinsdottir, M. Gonzalez, B. Kudisch, G. Galli, and D. Nocera "Oxidation chemistry of bicarbonate and peroxy carbonate: Implications for carbonate management in energy storage," *J. Am. Chem. Soc.*, *Accepted* (2023)
4. **Y. Shin** and G. Galli, "Tunable ferroelectricity in oxygen-deficient perovskites in Grenier structure," *under review* (2023) *ArXiv: 2307.04972* [[link](#)]
5. D. Shin, M. Lai, **Y. Shin**, J. S. Du, L. Jibril, J. M. Rondinelli, and C. A. Mirkin, "From heterostructures to solid-solutions: Structural tunability in mixed halide perovskites," *Advanced Materials*, **35**, 2205923 (2023) [[link](#)]
6. **Y. Shin** and J. M. Rondinelli, "Magnetic structure of oxygen-deficient nickelates perovskite with ordered vacancies," *Phys. Rev. Research*, **4**, L022069 (2022) [[link](#)]
7. **Y. Shin** and J. M. Rondinelli, "Strain-induced magnetic transitions in  $\text{SrMO}_{2.5}$  ( $M = \text{Mn, Fe}$ ) thin films with ordered-oxygen vacancies," *Inorganic Chemistry*, **60**, 13161 (2021) [[link](#)]
8. J. Wang, **Y. Shin**, J. R. Paudel, J. D. Grassi, R. K. Sah, W. Yang, E. Karapetrova, A. Zaidan, V. N. Strocov, C. Klewe, P. Shafer, A. X. Gray, J. M. Rondinelli, and S. J. May, "Strain-induced anion-site occupancy in perovskite oxyfluoride films," *Chemistry of Materials*, **33** (5) 1811-1820 (2020) [[link](#)]
9. **Y. Shin** and J. M. Rondinelli, "Pressure effects on magnetism in  $\text{Ca}_2\text{Mn}_2\text{O}_5$ -type ferrites and manganites," *Phys. Rev. B*, **102**, 10 (2020) [[link](#)]

10. J. Wang, **Y. Shin**, N. Gauquelin, Y. Yang, C. Lee, D. Jannis, J. Verbeeck, J. M. Rondinelli, and S. J. May, "Physical properties of epitaxial  $\text{SrMnO}_{2.5-\delta}\text{F}_\gamma$  oxyfluoride films," *Journal of Physics: Condensed Matter*, **31**, 365602 (2019) [[link](#)]
11. J. Wang, **Y. Shin**, E. Arenholz, B. M. Lefler, J. M. Rondinelli, and S. J. May, "Effect of fluoropolymer composition on topochemical synthesis of  $\text{SrMnO}_{3-\delta}\text{F}_\gamma$  oxyfluoride films," *Phys. Rev. M*, **2**, 073407 (2018) [[link](#)]
12. **Y. Shin** and J. M. Rondinelli, "Tunable band structures in digital oxides with layered crystal habits," *Phys. Rev. B*, **96**, 195108 (2017) [[link](#)]
13. **Y. Shin**, W.-S. Jung, and Y.-S. Lee, "First-principles study on the thermal expansion of Ni-X binary alloys based on the quasi-harmonic Debye model," *Metals and Materials International*, **22**, 1065-1072 (2016) [[link](#)]
14. **Y. Shin**, W. H. Cheung, T. T.M. Ho, K. E. Bremmell and D. A. Beattie, "Insights into hydrophobic molecule release from polyelectrolyte multilayer films using *in situ* and *ex situ* techniques," *Phys. Chem. Chem. Phys.* **16**, 22409 (2014) [[link](#)]

## PRESENTATIONS

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1. Oral: **Y. Shin** and G. Galli, "Ferroelectricity in oxygen-deficient ferrite perovskites," *American Physical Society March Meeting* (March 7, 2023)
2. Oral: **Y. Shin** and J. M. Rondinelli, "Magnetic structure of perovskite-derived  $\text{LaNiO}_{3-\delta}$  nickelate with ordered oxygen vacancies", *American Physical Society March Meeting* (Virtual; March 17, 2021)
3. Poster: **Y. Shin**, J. M. Rondinelli, "Electronic and magnetic transitions in  $\text{LaNiO}_{3-\delta}$  nickelate perovskites with ordered oxygen vacancies", *Materials Research Society Fall Meeting*, Boston, MA (December 2, 2019)
4. Oral: **Y. Shin**, J. M. Rondinelli, "Strain-induced magnetic transitions in  $\text{Sr}_2\text{Mn}_2\text{O}_5$  structure", *Materials Research Society Spring Meeting*, Phoenix, AZ (April 23, 2019)
5. Oral: **Y. Shin**, J. M. Rondinelli, "Pressure-induced magnetic behavior in  $\text{Ca}_2\text{Mn}_2\text{O}_5$ -type  $\text{A}_2\text{B}_2\text{O}_5$  oxides", *American Physical Society March Meeting*, Boston, MA (March 6, 2019)
6. Oral: **Y. Shin**, J. M. Rondinelli, "Band gap modulation via internal electric field control in Ruddlesden-Popper oxides", *American Physical Society March Meeting*, Los Angeles, CA (March 8, 2018)
7. Oral: **Y. Shin**, J. M. Rondinelli, "Strain-stabilization of novel magnetic orderings in  $\text{A}_2\text{B}_2\text{O}_5$  brownmillerite oxides", *Materials Research Society Fall meeting*, Boston, MA (November 28, 2017)
8. Poster: **Y. Shin**, J. M. Rondinelli, "Controlling Band Structure in Digital Oxides with Cation Order", *Center for Nanoscale Materials 10<sup>th</sup> Anniversary Symposium*, Lemont, IL (October 27, 2017)
9. Poster: **Y. Shin**, J. M. Rondinelli, "Tunable Band Gaps in digital oxides with layered crystal habits", *International Workshop on Oxide Electronics*, Chicago, IL (September 25, 2017)
10. Poster: **Y. Shin**, J. M. Rondinelli, "Tunable Band Gaps in digital oxides with layered crystal habits", *Northwestern Computational Research Day 2017*, Evanston, IL (April 18, 2017)

11. Oral: Y. Shin, J. M. Rondinelli, “Understanding the A-Cation Order Dependent Band Gap Variation in Ruddlesden-Popper Oxide”, *American Physical Society March Meeting*, New Orleans, LA (March 16, 2017)
12. Oral: Y. Shin, J. M. Rondinelli, “Understanding the A-Cation Order Dependent Band Gap Variation in Ruddlesden-Popper Oxide”, *Electronic Materials and Applications*, Orlando, FL (January 20, 2017)
13. Poster: Y. Shin, J. M. Rondinelli, “Understanding the A-Cation Order Dependent Band Gap Variation in Ruddlesden-Popper Oxide”, *Center for Atomic-scale Materials Design*, Copenhagen, Denmark (August 16, 2016)
14. Poster: Y. Shin, Y.-S. Lee, “Insights into the Effects of Elements on Thermal Expansion Behavior of Ni-based Superalloy using Density Functional Theory”, *Korean Institute of Metals and Materials*, Changwon, Korea (April 24, 2015)

## PROFESSIONAL SERVICE & OUTREACH

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<u>Teaching Assistant</u> for “Structure of Crystalline and Noncrystalline Materials”	Fall 2019
<u>Teaching Assistant</u> for “Topics on Solid State: Functional and Multifunctional Materials”	Fall 2017
<u>Participant</u> , Center for Atomic-scale Materials Design Summer School, Denmark	Aug 2016
<u>Operated proposal work</u> for supercomputer allocations Argonne National Lab and NSF	2016-2020
<u>Volunteer service</u> , at U.S.-Korea Conference on Science, Technology and Entrepreneurship	Aug 2019
<u>Volunteer service</u> , at KSEA National Math and Science Competition	Mar 2018
<u>Volunteer service</u> , teaching science classes in primary school in Vietnam	Feb 2011
<u>Volunteer service</u> at the International Percussion Festival in Seoul (IPFS)	July 2010
<u>Participant</u> , Youth Forum for 2 <sup>nd</sup> World Conference on Arts Education held by UNESCO	May 2010
<u>Piano club member</u> , Talk Through Piano (TTP) at Korea University Director of regular concert (2013)	2009 – 2014

## SKILLS

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### Computing Skills

Language	Python, Fortran 77/90/95, C programming, MATLAB, Shell script, AWK
Machine Learning	Scikit-learn, Pytorch, Tensorflow

### Language Skills

Certificate	Certificate of Translation Competence in Science and Technology, Korean Society of Translation
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