Curriculum Vitae (Dr Suhyun Yoo)

Suhyun Yoo, Ph.D.

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Date of Birth: 25th January 1988
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Education

2015 ~ 2020 **Ph. D.** in Mechanical Engineering, Ruhr-Universität Bochum, Bochum, Germany
- Dissertation: "Development of a Computational Framework to Determine the Chemical and Thermodynamic Stability of Electrode Materials in an Electrochemical Environment"
- Funded by the Cluster of Excellence RESOLV (EXC 2033) funded by the Deutsche Forschungsgemeinschaft
- **Awarded honor (Magna cum laude)** (2020)

2013 ~ 2015 **M. Sc.** in Materials Science and Engineering, Yonsei University, Seoul, Republic of Korea
- Dissertation: "An Ab Initio Study of Environment-dependent Nanomorphology of Palladium"
- Overall GPA **3.86/4.30**

2006 ~ 2013 **B. Sc.** in Materials Science and Engineering, Yonsei University, Seoul, Republic of Korea
- Dissertation: "Structural Properties and Electronic Structure of Zn_3N_2: A DFT Study and Beyond"
- Overall GPA: **3.85/4.30**

Professional Experience

2022/07 ~ present **Postdoctoral researcher** at Imperial College London, London, United Kingdom
- Department of Materials
- Job title: MSCA E4F Individual Fellow
- Topic: Lattice Polarisation Engineering for Next-Generation Photovoltaics
- Funded by the Marie Skłodowska-Curie Individual Fellowships

2022/05 ~ 2023/06 **Guest researcher** at Max-Planck-Insitut für Eisenforschung GmbH, Düsseldorf, Germany

2022/05 ~ 2022/06 **Postdoctoral researcher** at Department of Materials Science and Engineering, Yonsei University, Seoul, South Korea

2020/03 ~ 2022/04 **Postdoctoral researcher** at Max-Planck-Insitut für Eisenforschung GmbH, Düsseldorf, Germany
- Department of Computational Materials Design, Growth modelling group
- Topic: Addressing failure and degradation mechanisms of GaN based power electronics
- Funded by the ECSEL Joint Undertaking (JU) project UltimateGaN co-financed by EU and BMBF

2015/03 ~ 2020/03 **Ph. D. student** at Max-Planck-Insitut für Eisenforschung GmbH, Düsseldorf, Germany
- Department of Computational Materials Design, Electrochemistry and Corrosion group

- Topic: Development of a Computational Framework to Determine the Chemical and Thermodynamic Stability of Electrode Materials in an Electrochemical Environment
- Advisor: Prof Jörg Neugebauer

2017/03 ~ 2017/06 **Visiting researcher** at the University of California, Santa Barbara, USA

- Topic: Effect of spontaneous polarization of the wurtzite surfaces on its energetics and electronic structures
- Advisor: Prof Chris van de Walle

2014/01 ~ 2014/02 **Visiting researcher** at University of Bath, Bath, UK

- Topic: Identification of critical stacking faults in thin-film CdTe solar cells
- Advisor: Prof Aron Walsh

2011 ~ 2012 **Internship** in the Materials Theory Group, Yonsei University, Seoul, Korea

- Topic: Final-year thesis project "Structural properties and electronic structure of Zn_3N_2: A DFT study and beyond"
- Advisor: Prof Aloysius Soon

Awards & Honors

2022	**Finalist for the Gerhard Ertl Young Investigator Award,** Sponsor: The journal Surface Science, Elsevier Scientific Publishing
2021/11/26	**Energy for Future (E4F) postdoctoral fellowship,** an initiative of the Horizon 2020 MSCA-COFUND Program coordinated by Fundación Iberdrola España
2020/03/15	**Academic Excellence Award (Magna cum laude)**, Department of Mechanical Engineering, Ruhr-Universität Bochum, Bochum, Germany
Spring, 2014	**Awarded BK21 Plus Participation Scholarship**, Yonsei University, Seoul, Korea
Fall, 2013	**Awarded Global Partner Research Scholarship**, Department of Chemistry, University of Bath, Bath, UK
Fall, 2013	**Awarded BK21 Plus Participation Scholarship**, Yonsei University, Seoul, Korea
Spring, 2013	**Awarded Yonsei Alumni Scholarship**, Yonsei University, Seoul, Korea
Fall, 2012	**Academic Excellence Award**, Department of Materials Science and Engineering, Yonsei University, Seoul, Korea
Fall, 2011	**Academic Excellence Award**, Department of Materials Science and Engineering, Yonsei University, Seoul, Korea

Research Interests & Skills

My research focus is on ab-initio investigations of solid-state materials and their surface phenomena. Employing ab-initio electronic structure calculations with high-performance computing, I studied

- environment-dependent stabilization mechanisms of semiconductor surfaces
- development of a novel methodology correctly describing the effect of polarization in ab-initio surface calculations
- impurity incorporation mechanisms in metal nanostructures
- an impact of planar defects in photovoltaic materials on energetics and electronic structure.

Currently, I have investigated the failure and degradation mechanisms of GaN-based electronics with accounting for the defect-related properties since 2020.

A major strength of my research skills is to investigate surface phenomena such as impacts surface defects and morphology of semiconductors exhibiting polarization have on its energetics and electronic structure, based on quantum mechanical ab-initio calculations [e.g., using Vienna Ab initio Simulations Package (VASP) code], knowledge of semiconductor physics and surface science, and computing skills (e.g., python and shell scripting) to perform high-throughput calculations. I have actively worked with theoretical and experimental collaborators based in Germany, the Republic of Korea, and the USA to provide atomistic insights into various projects such as growth mechanism of nanoparticles and discovery of potential neuromorphic materials.

Publications in peer-reviewed scientific journals

Summary: 15 articles / first-author articles: 13 and corresponding-author articles: 5

[§]: First Author/*: Corresponding Author

15	**2022**	S.-H. Kim[§,*], **S.-H. Yoo**[§], S. Shin, A. A. El-Zoka, O. Kasian, J. Lim, J. Jeong, C. Scheu, J. Neugebauer, H. Lee, M. Todorova, B. Gault*, "Controlled doping of electrocatalysts through engineering impurities"	***Adv. Mater.*** 2203030 (2022) – IF[#]: 30.849
14	**2022**	(1 citation) S.-H. Kim[§,*], **S.-H. Yoo**[§,*], P. Chakraborty, J. Jeong, J. Lim, A. A. El-Zoka, L. T. Stephenson, T. Hickel, J. Neugebauer, C. Scheu, M. Todorova, B. Gault[*], "Understanding Alkali Contamination in Colloidal Nanomaterials to Unlock Grain Boundary Impurity Engineering"	***J. Am. Chem. Soc.*** 144, 2, 987-994 (2022) – IF: 14.612
13	**2022**	(1 citation) **S.-H. Yoo**[§,*], S.-H. Kim, E. Woods, B. Gault*, M. Todorova, and J. Neugebauer, "Origin of the hydrogen Signal in Atom Probe Tomography: Case Studies of Alkali and Noble Metals"	***New J. Phys.*** 24, 013008 (2022) – IF: 3.732
12	**2021**	W. Hwang[§], **S.-H. Yoo**[§], A. Soon*, and W. Jang*, "Going Beyond the Equilibrium Crystal Shape: Re-tracing the Morphological Evolution in Group 5 Tetradymite Nanocrystals"	***Nanoscale*** 13, 15721-15730 (2021) – IF: 7.790
11	**2021**	(2 citation) **S.-H. Yoo**[§], Y. Na, W. Hwang, W. Jang*, and A. Soon*, "First-Principles Calculations of Heteroanionic Monochalcogenide Alloy Nanosheets with Direction-dependent Properties for Anisotropic Optoelectronics"	***ACS Appl. Nano Mater.*** 4, 6, 5912–5920 (2021) – IF: 5.097
10	**2021**	(6 citations) **S.-H. Yoo**[§,*], M. Todorova*, D. Wickramaratne, L. Weston, C. G. Van de Walle, and J. Neugebauer, "Finite-Size Correction for Slab Supercell Calculations of Materials with Spontaneous Polarization"	***npj Comput. Mater.*** 7, 58 (2021) – IF: 12.241
9	**2021**	**S.-H. Yoo**[§,*], L. Lymperakis, and J. Neugebauer, "Efficient Electronic Passivation Scheme for Computing Low-Symmetry Compound Semiconductor Surfaces in Density-Functional Theory Slab Calculations"	***Phys. Rev. Mater.*** 5, 044605 (2021) – IF: 3.989
8	**2021**	(2 citations) Y.-J. Lee[§], M. Han[§], **S.-H. Yoo***, and A. Soon*, "Tunable Threshold Voltage of ZnTe-Based Ovonic Switching Devices via Isovalent Cation Exchange"	***ACS Appl. Electron. Mater.*** 3, 1107-1114 (2021) – IF: 3.314

7	**2019**	(8 citations) **S.-H. Yoo**§, N. Siemer, M. Todorova*, D. Marx and J. Neugebauer, "Deciphering Charge Transfer and Electronic Polarization Effects at Gold Nanocatalysts on Reduced Titania Support"	***J. Phys. Chem. C*** 123, 5495 (2019) – IF: 4.126
6	**2018**	(18 citations) **S.-H. Yoo**§, M. Todorova*, and J. Neugebauer, "Selective Solvent-Induced Stabilization of Polar Oxide Surfaces in an Electrochemical Environment"	***Phys. Rev. Lett. (Editor's suggestion),*** 120, 066101 (2018) – IF: 9.161
5	**2017**	(4 citation) C. E. Kim§, **S.-H. Yoo,** D. F. Bahr, C. Stampfl, and A. Soon*, "Uncovering the Thermo-Kinetic Origins of Phase Ordering in Mixed-Valence Antimony Tetroxide by First-Principles Modeling"	***Inorg. Chem.*** 56, 6645 (2017) – IF: 5.165
4	**2016**	(30 citations) **S.-H. Yoo**§, J.-H. Lee, Y.-K. Jung, and A. Soon*, "Exploring Stereographic Surface Energy Maps of Cubic Metals via an Effective Pair-Potential Approach"	***Phys. Rev. B***, 93, 035434 (2016) – IF: 4.036
3	**2014**	(53 citations) **S.-H. Yoo**§, K. T. Butler, A. Soon, A. Abbas, J. M. Walls*, and A. Walsh*, "Identification of Critical Stacking Faults in Thin-Film CdTe Solar Cells"	***Appl. Phys. Lett.*** 105, 062104 (2014) – IF: 3.791
2	**2014**	(22 citations) **S.-H. Yoo**§, J.-H. Lee, B. Delley, and A. Soon*, "Why Bromine Squares Palladium off? An Ab Initio Study of Brominated Palladium and Its Nano Morphology"	***Phys. Chem. Chem. Phys.*** 16, 18570 (2014) – IF: 3.676
1	**2014**	(43 citations) **S.-H. Yoo**§, A. Walsh*, D. O. Scanlon, and A. Soon*, "Electronic Structure and Band Alignment of Zinc Nitride, Zn_3N_2"	***RSC Adv.*** 4, 3306 (2014) – IF: 3.361

#: Impact factors (IF) of journals released in Journal Citation Reports in 2020

Oral Presentations

Summary: 10 oral presentations in international scientific conferences/ 9 invited talks

18	**Invited 2022/06/02**	**S.-H. Yoo** "Surface investigation of semiconductors exhibiting spontaneous polarization & Impurity incorporation in Pd nanomaterials"	Colloquium in Korea Institute of Energy Research (KIER), Republic of Korea
17	**Invited 2022/05/17**	**S.-H. Yoo** "Brief introduction to density-functional theory & Alkali impurity incorporation in Pd nanomaterials"	Lab seminar of Energy Materials Lab, Incheon National University, Republic of Korea
16	**Invited 2022/05/10**	**S.-H. Yoo** "Deciphering charge transfer at Au catalysts on TiO_2 surfaces and alkali impurity incorporation in Pd nanomaterials"	Colloquium in KITECH Busan, Republic of Korea
15	**Invited 2022/04/22**	**S.-H. Yoo**, M. Todorova, L. Lymperakis, C. Van de Walle, and J. Neugebauer "Efficient electronic passivation schemes for surface calculations of semiconductors exhibiting spontaneous polarization: Thermodynamic and electronic properties of GaN surfaces"	2022 Korean Physical Society Spring meeting, Republic of Korea (online conference)
14	**Invited 2022/04/08**	**S.-H. Yoo**, "Impurity-incorporation mechanisms in Pd Nanoaerogels and metals"	Lab seminar of the Materials Theory Group, Department of Materials Science and

			Engineering, Yonsei University, Seoul, Republic of Korea
13	**Invited 2021/12/09**	**S.-H. Yoo,** "Identifying impurity incorporation mechanisms in metal nanostructures: A first-principles approach"	2021 Kosen Bridge Forum, Online seminar (organized by KIST), Republic of Korea
12	**Invited 2021/10/03**	**S.-H. Yoo,** "Overcoming Failing Size Convergence for Surface Calculations of Materials Exhibiting Spontaneous Polarization"	Materials Oceania 2021: Materials Science and Engineering, Australia
11	**Invited 2021/04/26**	**S.-H. Yoo,** "Electronic passivation schemes for surfaces with spontaneous polarization and for low symmetry semiconductor surfaces in DFT slab calculations"	Lab seminar of the Materials Design Group, Department of Materials, Imperial College London, London, UK
10	**Contributed 2021/03/01**	**S.-H. Yoo**, M. Todorova, D. Wickramaratne, L. Weston, C. G. Van de Walle, and J. Neugebauer, "Enabling and Boosting Size Convergence for Surface Calculations of Materials Exhibiting Spontaneous Polarization"	Spring Meeting of the German Physical Society (DPG 2021), Germany
9	**Contributed 2020/11/27**	**S.-H. Yoo**, M. Todorova, D. Wickramaratne, L. Weston, C. G. Van de Walle, and J. Neugebauer, "Enabling and Boosting Size Convergence for Surface Calculations of Materials Exhibiting Spontaneous Polarization"	2020 MRS Fall Meeting & Exhibit, Boston, USA (online participation)
8	**Invited 2020/11/19**	**S.-H. Yoo,** "Investigations of materials surfaces based on density functional theory calculations"	Invited talk, Department seminar, Department of Chemistry in Kangwon University, Chuncheon, Republic of Korea
7	**Contributed 2020/11/03**	**S.-H. Yoo**, M. Todorova, D. Wickramaratne, L. Weston, C. G. Van de Walle, and J. Neugebauer, "Enabling and Boosting Size Convergence for Surface Calculations of Materials Exhibiting Spontaneous Polarization"	Electronic Materials and Nanotechnology for Green Environment (ENGE), Jeju, Republic of Korea
6	**Contributed 2019/04/02**	**S.-H. Yoo**, N. Siemer, M. Todorova, D. Marx and J. Neugebauer, "Impact of the Oxygen Vacancies on Au Nano-Clusters Supported on Reduced TiO_2(110) Surface"	Spring Meeting of the German Physical Society (DPG 2019), Regensburg, Germany
5	**Contributed 2018/03/14**	**S.-H. Yoo**, M. Todorova, and J. Neugebauer, "Selective Solvent-Induced Stabilization of Polar Oxide Surfaces in An Electrochemical Environment"	Spring Meeting of the German Physical Society (DPG 2018), Berlin, Germany
4	**Contributed 2017/03/16**	**S.-H. Yoo**, M. Todorova, and J. Neugebauer, "An Ab-Initio Study on The Stability of ZnO(0001)-Zn Surfaces in An Electrochemical Environment"	American Physical Society (APS) March Meeting 2017, New Orleans, USA (2017)
3	**Contributed 2016/11/08**	**S.-H. Yoo**, M. Todorova, and J. Neugebauer, "A First-Principles Study on the Phase Stability of ZnO(0001)-Zn Surfaces in an Electrochemical Environment"	Electronic Materials and Nanotechnology for Green Environment (ENGE), Jeju, Republic of Korea
2	**Contributed 2016/03/11**	**S.-H. Yoo**, M. Todorova, and J. Neugebauer, "A First-Principles Study on The Phase Stability of ZnO(0001)-Zn Surfaces"	Deutsche Physikalische Gesellschaft e.V (DPG), Regensburg, Germany
1	**Contributed 2013/10/25**	**S.-H Yoo**, A. Walsh, D. O. Scanlon, and A. Soon, "Electronic Structure and Band Alignment of Zinc Nitride, Zn_3N_2"	The Korean Institute of Metals and Materials conference (KIM), Gwang-ju, Republic of Korea

Poster Presentations

Summary: 5 poster presentations in international scientific conferences

8	**Contributed 2021/12/08**	**S.-H. Yoo**, L. Limperakis, and J. Neugebauer, "Thermodynamics and Growth of V-pit Defects on Wurtzite GaN Polar Surfaces"	2021 MRS Fall Meeting & Exhibit, Boston, USA (online participation)
7	**Contributed 2017/11/27**	**S.-H. Yoo**, M. Todorova, and J. Neugebauer, "An Ab-Initio Study on The Stability of ZnO(0001)-Zn Surfaces in An Electrochemical Environment"	Electrochemistry Workshop: The Electrode Potential in Electrochemistry – A Challenge for Electronic Structure Theory Calculations, Reisensburg, Germany
6	**Contributed 2015/09/07**	**S.-H. Yoo**, M. Todorova, and J. Neugebauer, "Stability of Zinc Oxide (0001) Surface in An Electrochemical Environment – An Ab Initio Study"	Psi-k Conference, San Sebastian-Donostia, Spain
5	**Contributed 2014/11/04**	**S.-H. Yoo**, A. Walsh, D. O. Scanlon, and A. Soon, "Electronic Structure and Band Alignment of Zinc Nitride, Zn_3N_2"	The 17th Asian Workshop on First-Principles Electronic Structure Calculations, Seoul, Republic of Korea
4	**Contributed 2014/07/07**	**S.-H. Yoo**, K. T. Butler, A. Soon, A. Abbas, J. M. Walls and A. Walsh, "Identification of Critical Stacking Faults in Thin-Film CdTe Solar Cells"	Centre for Sustainable Chemical Technologies Summer Showcase, University of Bath, Bath, UK
3	**Contributed 2013/12/11**	**S.-H. Yoo**, A. Walsh, D. O. Scanlon, and A. Soon, "Electronic Structure and Band Alignment of Zinc Nitride, Zn_3N_2"	The 8th International Conference on Advanced materials and Devices (ICAMD), Jeju, Republic of Korea
2	**Contributed 2013/10/25**	**S.-H Yoo**, J.-H Lee, B. Delley, and A. Soon, "Why Bromine Squares Palladium off? An Ab Initio Study of Brominated Palladium and Its Nano Morphology"	Electronic Materials and Nanotechnology for Green Environment (ENGE), Gwang-ju, Republic of Korea
1	**Contributed 2013/09/16**	**S.-H Yoo**, A. Walsh, D. O. Scanlon, and A. Soon, "Electronic Structure and Band Alignment of Zinc Nitride, Zn_3N_2"	Centre for Sustainable Chemical Technologies Summer Showcase, University of Bath, Bath, UK

Supervising

2021 **Co-supervising** 1 Master student in Materials Theory Group (by Prof. Aloysius Soon) in Yonsei University, Seoul, Republic of Korea as an affiliated research associate

Military Service

2007 ~ 2009 **Honorable discharge as a sergeant in Republic of Korea Air Force (ROKAF)**

- Served in Air Force's Chemical Corps.