In Won Yeu, Ph.D.

Curriculum Vitae (April 4, 2024)

Personal Data

Position:	Postdoctoral Research Scientist Chemical Engineering, Columbia University 613 Havemeyer Hall, 3000 Broadway, New York, NY 10027, United States Tel.) +1-201-562-2938
Email:	iy2185@columbia.edu (Primary) yiw0121@snu.ac.kr (Secondary)
Homepage:	https://inwonyeu.github.io
Date of Birth:	Jan 21, 1993
Nationality:	Republic of Korea
Marital Status:	Single
Language:	Korean (native), English
Military service:	Discharged

Education

03/2015 – 08/2020 **Ph.D.**, Materials Science and Engineering
Seoul National University (SNU), GPA 4.14/4.3
Seoul, Republic of Korea
Advisor: Prof. Cheol Seong Hwang and Dr. Jung-Hae Choi
Thesis: "Computational Investigation on the Anisotropic Surface Structures and Growth of GaAs: from Ab Initio to Thermodynamics"

03/2011 – 02/2015 **B.S.** *summa cum laude*, Materials Science and Engineering
Seoul National University (SNU), GPA 3.96/4.3 (**Major GPA** 4.07/4.3)
Seoul, Republic of Korea

Professional Experiences

09/2021 – present **Postdoctoral Research Scientist**, Chemical Engineering & Columbia Center for Computational Electrochemistry (CCCE), **Columbia University**
New York, United States
Advisor: Prof. Alexander Urban

10/2020 – 08/2021 **Postdoctoral Researcher**, Electronic Materials Research Center
Korea Institute of Science and Technology (KIST)
Seoul, Republic of Korea
Advisor: Dr. Jung-Hae Choi

Research Interests

✓ **Computational materials science**

- Materials modeling based on Density Functional Theory and Machine Learning to explore process-structure-property-performance relationships
- Bottom-up approaches bridged by crystallographic symmetry, statistical mechanics, and nucleation theory: from first-principles to thermodynamics/kinetics
- Development of computational methodology and its implementation in automation software
- Leveraging the numerical methods of crystallography, machine learning, and graph theory into computational materials design

✓ **Atomistic understanding of spontaneous formation of nanostructure morphology**

- Understanding the formation principle of atomic structures depending on process conditions
- Predicting the anisotropic interaction between solid surfaces and their environments
- Elucidating the peculiar unidirectional growth morphology of dendrite and nanowires

✓ **Material implications for device characteristics**

- Polar materials: III-V and II-VI for optoelectronics, $(Hf,Zr)O_2$ for ferroelectrics, $SrTiO_3$ for high-k and resistance-switching materials
- SnO for p-type oxide semiconductors
- Solid electrolyte interphase (SEI) and Li dendrite formed by Anode/electrolyte interface reactions in Li metal batteries

Technical Skills

✓ **Theoretical background**

- Statistical mechanics and thermodynamic modeling
- Atomistic modeling of interface chemical process and its implications for materials growth
- Electronic structure and semiconductor device physics
- Development and Application of machine learning potentials for materials
- Interface phonon computation
- Computational crystallography/group theory

✓ **Simulation software**

- Density functional theory: **VASP** (primary), **FHI-aims** (for core orbital calculations like XPS binding energy), **CASTEP** (for NMR simulations), **Quantum ESPRESSO**
- Deep learning: **TensorFlow**, **Keras**, **PyTorch**
- Scientific open-source package: **ASE**, **Pymatgen**, **ænet, ænet-PyTorch**, **Phonopy**, **Spglib**

✓ **Programming language**

- **Python** (expert)
- **MATLAB** (expert)
- **C & C++** (intermediate)
- **HTML/CSS** (intermediate)

Developed Codes

GPR-ANN (Python) A Package for ANN Interatomic Potentials accelerated by Gaussian Process Regression (GPR)
Source Code: to be released, https://github.com/atomisticnet/??
Paper: in preparation

InterPhon (Python) A Package for Ab initio Interface Phonon Calculations
Source Code: https://github.com/inwonyeu/interphon
Manual: https://interphon.readthedocs.io
Paper: https://doi.org/10.1016/j.cpc.2021.108089

Publications

[22] Taeyoung Jeong, **In Won Yeu**, Kun Hee Ye, Seungjae Yoon, Dohyun Kim, Cheol Seong Hwang*, and Jung-Hae Choi*

"Study of Charge Transition-Driven Resistive Switching Mechanism in TiO_2-based Random Access Memory via Density Functional Theory"
***Nanoscale*, https://doi.org/10.1039/d3nr06614b**

[21] Kun Hee Ye, **In Won Yeu**, Gyuseung Han, Taeyoung Jeong, Seungjae Yoon, Dohyun Kim, Cheol Seong Hwang*, and Jung-Hae Choi*

"Comprehensive interpretations of thermodynamic and kinetic effects on the phase fractions in $Hf_{1-x}Zr_xO_2$ by first principle calculations"
***Applied Physics Reviews* 10, 031419 (2023)**

[20] Narendra S. Parmar, Haena Yim, Lynn A. Boatner, Panithan Sriboriboon, Yunseok Kim, Kyung Song, Jung-Hae Choi, **In Won Yeu**, and Ji-Won Choi*

"Ordered Electronic Reconstruction of the (11-20) ZnO Single Crystal"
***Advanced Electronic Materials* 9, 2201336 (2023)**

[19] Jon López-Zorrilla, Xabier M. Aretxabaleta, **In Won Yeu**, Iñigo Etxebarria, Hegoi Manzano, and Nongnuch Artrith*

"ænet-PyTorch: a GPU-supported implementation for machine learning atomic potentials training"
***Journal of Chemical Physics* 158, 164105 (2023)**

[18] Gyuseung Han, **In Won Yeu**, Kun Hee Ye, Seungjae Yoon, Taeyoung Jeong, Seung-Cheol Lee, Cheol Seong Hwang, and Jung-Hae Choi*

"Temperature-dependent bandgap of (In,Ga)As via P5Grand: a Python Package for Property Prediction of Pseudobinary systems using Grand canonical ensemble"
***Chemical Physics Letters* 804, 139887 (2022)**

[17] Haengha Seo, **In Won Yeu**, Dae Seon Kwon, Dong Gun Kim, Junil Lim, Tae Kyun Kim, Heewon Paik, Jung-Hae Choi*, and Cheol Seong Hwang*

"The Contrasting Impacts of the Al_2O_3 and Y_2O_3 Insertion Layers on the Crystallization of ZrO_2 Films for Dynamic Random Access Memory Capacitors"

***Advanced Electronic Materials* 8, 2200099 (2022)**

[16] Gyuseung Han, **In Won Yeu**, Kun Hee Ye, Cheol Seong Hwang, and Jung-Hae Choi*

"Atomistic prediction on the composition- and configuration- dependent bandgap of Ga(As,Sb) using cluster expansion and *ab initio* thermodynamics"

***Materials Science and Engineering B* 280, 115713 (2022)**

[15] **In Won Yeu**, Gyuseung Han, Kun Hee Ye, Cheol Seong Hwang, and Jung-Hae Choi*

"*InterPhon*: *Ab initio* Interface Phonon Calculations within a 3D Electronic Structure Framework"

***Computer Physics Communications* 268, 108089 (2021)**

[14] Hansung Kim, **In Won Yeu**, Gyuseung Han, Gunwu Ju, Yun Joong Lee, Young-hun Shin, Jung-Hae Choi, Hyun Cheol Koo*, and Hyung-jun Kim*

"Surface Morphology Evolution and Underlying Defects in Homoepitaxial Growth of GaAs (110)"

***Journal of Alloys and Compounds* 874, 159848 (2021)**

[13] Kun Hee Ye, Gyuseung Han, **In Won Yeu**, Cheol Seong Hwang*, and Jung-Hae Choi*

"Atomistic Understanding of the Ferroelectric Properties of a Wurtzite Structure (AlN)n/(ScN)m Superlattice"

***Phys. Status Solidi RRL* 15, 2100009 (2021)**

[12] Gyuseung Han, **In Won Yeu**, Kun Hee Ye, Seung-Cheol Lee, Cheol Seong Hwang*, and Jung-Hae Choi*

"Atomistic prediction on the configuration- and temperature-dependent dielectric constant of $Be_{0.25}Mg_{0.75}O$ superlattice as a high-κ dielectric layer"

***Journal of Materials Chemistry C* 9, 851 (2021), Inside Front Cover**

[11] Gyuseung Han, **In Won Yeu**, Jaehong Park, Kun Hee Ye, Seung-Cheol Lee, Cheol Seong Hwang, and Jung-Hae Choi*

"Effect of local strain energy to predict accurate phase diagram of III-V pseudobinary systems: case of Ga(As,Sb) and (In,Ga)As"

***Journal of Physics D: Applied Physics* 54, 045104 (2021)**

[10] **In Won Yeu**, Gyuseung Han, Cheol Seong Hwang, and Jung-Hae Choi*

"An *ab initio* approach on the asymmetric stacking of GaAs <111> nanowires grown by a vapor-solid method"
***Nanoscale* 12, 17703 (2020), Outside Front Cover**

[9] Kai Liu, **In Won Yeu**, Cheol Seong Hwang, and Jung-Hae Choi*
"Initial oxidation and surface stability diagram of Ge(100) as a function of the temperature and oxygen partial pressure through ab-initio thermodynamics"
***Physica Scripta* 95, 025701 (2020)**

[8] Jaehong Park, **In Won Yeu**, Gyuseung Han, Cheol Seong Hwang, and Jung-Hae Choi*
"Ferroelectric switching in bilayer 3R MoS_2 via interlayer shear mode driven by nonlinear phononics"
***Scientific Reports* 9, 14919 (2019)**

[7] **In Won Yeu**, Gyuseung Han, Jaehong Park, Cheol Seong Hwang, and Jung-Hae Choi*
"Theoretical understanding of the catalyst-free growth mechanism of GaAs <111>B nanowires"
***Applied Surface Science* 497, 143740 (2019)**

[6] Younjin Jang†, **In Won Yeu**†, Jun Shik Kim, Jeong Hwan Han, Jung-Hae Choi*, and Cheol Seong Hwang* **(†: co-first authors)**
"Reduction of the Hysteresis Voltage in Atomic-layer-deposited p-Type SnO Thin-Film Transistors by Adopting Al_2O_3 Interfacial Layer"
***Advanced Electronic Materials* 5, 1900371 (2019)**

[5] Jaehong Park, **In Won Yeu**, Gyuseung Han, Chaun Jang, Joon Young Kwak, Cheol Seong Hwang, and Jung-Hae Choi*
"Optical Control of the Layer Degree of Freedom through Wannier-Stark States in Polar 3R MoS_2"
***Journal of Physics: Condensed Matter* 31, 315502 (2019)**

[4] Jaehong Park, **In Won Yeu**, Gyuseung Han, Cheol Seong Hwang, and Jung-Hae Choi*
"Role of the short-range order in amorphous oxide on MoS_2/a-SiO_2 and MoS_2/a-HfO_2 interfaces"
***Physica Status Solidi B* 256, 1900002 (2019)**

[3] **In Won Yeu**, Gyuseung Han, Jaehong Park, Cheol Seong Hwang, and Jung-Hae Choi*
"Equilibrium crystal shape of GaAs and InAs considering surface vibration and new (111)B reconstruction: ab-initio thermodynamics"
***Scientific Reports* 9, 1127 (2019)**

[2] **In Won Yeu**, Jaehong Park, Gyuseung Han, Cheol Seong Hwang, and Jung-Hae Choi*
"Surface reconstruction of InAs (001) depending on the pressure and temperature examined

by density functional thermodynamics"
***Scientific Reports* 7, 10691 (2017)**

[1] Woongkyu Lee, Sijung Yoo, Kyung Jean Yoon, **In Won Yeu**, Hye Jung Chang, Jung-Hae Choi, Susanne Hoffmann-Eifert, Rainer Waser, and Cheol Seong Hwang*
"Resistance switching behavior of atomic layer deposited $SrTiO_3$ film through possible formation of $Sr_2Ti_6O_{13}$ or $Sr_1Ti_{11}O_{20}$ phases"
***Scientific Reports* 6, 20550 (2016)**

International Conferences

11/30/2023 "Accelerating the Construction of ANN Interatomic Potentials Using Surrogate Models"
2023 MRS Fall Meeting and Exhibit (2023 MRS Fall), Boston, United States, Oral

11/09/2022 "Accelerating the Construction of ANN Interatomic Potentials Using Surrogate Models"
The 7th International Conference on Electronic Materials and Nanotechnology for Green Environment (ENGE 2022), Jeju, Republic of Korea, Oral

03/02/2021 "Atomistic Modeling for the Vapor-Phase Growth of GaAs Nanowires: from DFT to Growth Kinetics"
SurfaceScience21 (DPG Spring Meeting), Online, Germany, Poster

10/04/2020 "Atomistic Understanding on the Surface of GaAs By Ab Initio Thermodynamics; From Equilibrium Shape to Growth Shape"
Pacific Rim Meeting (PRiME 2020), Online, Oral (**invited**)

07/01/2020 "Effects of growth condition on the anisotropic growth and stacking behavior of GaAs polar nanowires: ab initio thermodynamics"
The 18th International Nanotech Symposium & Exhibition (Nano Korea 2020), Online & KINTEX, Republic of Korea, Oral

11/03/2019 "Prediction of the Surface Energy from the Robust Extraction of Local Energy via Atomic Neural Network"
The 5th International Conference on Molecular Simulation (ICMS 2019), Jeju, Republic of Korea, Poster

06/24/2019 "Growth mechanism of III-V nanowires depending on the temperature and pressure: ab-initio thermodynamic study"
EuroCVD 22-Baltic ALD 16, Luxexpo, Luxembourg, Poster

11/02/2018 "Equilibrium crystal shape of GaAs by ab-initio thermodynamics"
International Conference on Multiscale Materials Modeling (9th MMM2018), Osaka,

Japan, Oral

10/29/2018 "Vibrational effects on the surface energy of III-V compound semiconductors using ab-initio thermodynamics"
The 21st Asian Workhop on First-Principles Electronic Structure Calculations, Daejeon, Republic of Korea, Poster

08/19/2018 "Surface phase diagram of GaAs(001) considering the vibrational thermal energy by ab-initio calculation"
IUMRS-ICEM 2018, Daejeon, Republic of Korea, Oral

07/04/2016 "Oxygen Adsorption Behavior of InAs Nanowire by Ab-initio Calculations"
IUMRS-ICEM 2016, Suntec City, Singapore, Oral

09/06/2015 "Reconstruction structure of InAs surfaces and their effects on electronic structure"
Psi-K 2015, Donostia/San Sebastian, Spain, Poster

Domestic Conferences

01/28/2021 "Ab initio Approach on the Anisotropic Growth of GaAs: from DFT to Growth Kinetics"
The 28th Korean Conference on Semiconductors (KCS 2021), Oral

02/12/2020 "Atomistic Understanding on the Growth and Stacking-Fault of GaAs Nanowires Grown by Noncatalytic Method"
The 27th Korean Conference on Semiconductors (KCS 2020), Poster

07/04/2019 "Theoretical understanding on the growth and stacking-fault mechanism of GaAs nanowires grown by catalyst-free method"
The 15th KIAS Electronic Structure Calculation Workshop (ESCW2019), Poster

02/13/2019 "Effect of the two-dimensional strain on the equilibrium crystal shape of GaAs by ab-initio thermodynamics"
The 26th Korean Conference on Semiconductors (KCS 2019), Oral

06/21/2018 "Equilibrium crystal shape of GaAs and InAs by ab-initio thermodynamics"
The 14th KIAS Electronic Structure Calculation Workshop (ESCW2018), Poster

02/05/2018 "Surface reconstruction and equilibrium shape of III-V compound semiconductors as a function of pressure and temperature by ab-initio thermodynamics"
The 25th Korean Conference on Semiconductors (KCS 2018), Oral

06/15/2017 "Surface morphology of InAs considering entropy effects"
The 13th KIAS Electronic Structure Calculation Workshop (ESCW2017), Poster

02/13/2017 "DFT study on the clean-up mechanism of InGaAs(001) native oxides in atomic layer deposition"
The 24th Korean Conference on Semiconductors (KCS 2017), Oral

02/22/2016 "Oxidation Study on the (100), (110) and (111) Surfaces of InAs by ab-initio Calculations"
The 23th Korean Conference on Semiconductors (KCS 2016), Oral

06/18/2015 "Surface structure and surface energies of InAs"
The 11th KIAS Electronic Structure Calculation Workshop (ESCW2015), Poster

Honors and Awards

Doyeon academic paper award
Inter-university Semiconductor Research Center (ISRC),
Seoul National University, 2021

The 11th Semiconductor day scholarship award ($10,000)
Korea Semiconductor Industry Association (KSIA), 2017

Graduation with honors (summa cum laude)
Seoul National University, 2015

National science and engineering scholarship ($25,000)
Korea Student Aid Foundation (KOSAF), 2011-2014

References

1. Prof. Cheol Seong Hwang (Ph.D. Thesis Advisor)
Distinguished Professor
Dielectric Thin Film Laboratory
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Homepage: http://dtfl.snu.ac.kr
Email: cheolsh@snu.ac.kr

2. Dr. Jung-Hae Choi (Ph.D. Thesis Advisor)
Principal Research Scientist
Electronic Materials Research Center
Advanced Materials Research Division
Korea Institute of Science and Technology (KIST)
Phone: +82-2-958-5488
Homepage: https://sites.google.com/view/junghaechoi
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3. Prof. Sangtae Kim (Ph.D. Thesis Committee)
Assistant Professor
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