CURRICULUM VITAE

Hyun-Jung Kim

Ph.D.
Senior Research Engineer / Workstream Lead
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Professional Profile

Computational materials physicist and enterprise AI workstream lead with experience spanning **first-principles simulation**, **materials discovery**, and **AI governance**. At LG Display, I connect research depth with operational execution by supporting **AI project review**, **tech scouting**, and **internal AI capability building** in a security-constrained enterprise environment. My long-term research agenda focuses on integrating **AI/ML**, **generative models**, and **quantum optimization** into practical inverse-design workflows for molecular and materials discovery.

Education

Ph.D. in Theoretical Condensed Matter Physics (Hanyang University) Mar. 02 2011 - Aug. 21 2015
Advisor: Prof. Dr. Jun-Hyung Cho
Thesis title:"*Electronic properties of self-assembled low-dimensional nano-structures on surfaces*"

M.S. in Theoretical Condensed Matter Physics (Hanyang University) Mar. 02 2009 - Feb. 18 2011
Advisor: Prof. Dr. Jun-Hyung Cho
Thesis title: "*Length- and parity-dependent electronic states in one-dimensional carbon chains on C(111)*"

B.S. in Physics (Hanyang University) Feb. 27 2003 - Feb. 20 2009 (military service Jan. 6 2004 - Jan. 5 2006)
Thesis title: "*First-principles study of the structure and electronic properties of C(110) surface*"

Research & Industrial Experience

Industry positions

- **Sep. 05 2022 ∼ present : Senior Research Engineer / Workstream Lead**,
  AI/Big Data Research Division, AX Group, LG Display, Paju Complex 245, LG-ro, Wollong-myeon, Paju-si, 10845 Gyeonggi-do, Korea

  Role:
  - **OLED Materials Researcher(−2024):** Quantum-chemical/DFT-driven analysis for **molecular design** and **inverse-design** problem formulation; contributed to project-based R&D execution.
  - **AI Instructor (2025):** Delivered internal training on **"AI/ML Fundamentals"**, **workflow automation**, and **LLM application development**.
  - **Workstream Lead (AI Governance Team; current)**: leading **AI project review and portfolio management**, **tech scouting**, and **AI Tech Committee operations**; maturing

quantum-computing use cases into scoped pilot proposals and **external research collaborations**.

Academic positions

- **Aug. 01 2020 ∼ Jul. 31 2022 : Visiting Scientist (supported by Humboldt Research Fellowship)**,
  Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany
  Host: Prof. Stefan Blügel
- **Mar. 01 2020 ∼ Jul. 31 2020 : Postdoctoral researcher**,
  Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany
  Advisor: Prof. Stefan Blügel
- **Sep. 09 2019 ∼ Feb. 29 2020 : Research fellow**,
  Quantum Universe Center, Korea Institute for Advanced Study, Seoul, Korea
  Advisor: Prof. Young-Woo Son
- **Sep. 01 2015 ∼ Aug. 31 2019 : Postdoctoral researcher**,
  School of Computational Sciences, Korea Institute for Advanced Study, Seoul, Korea
  Advisor: Prof. Young-Woo Son

Mentoring & Academic Service

- **M.Sc. thesis co-supervision (RWTH Aachen University / Forschungszentrum Jülich)**,
  Xiaoyu Liu, *"Electronic Structure of Twisted Bilayer Tungsten Diselenide investigated by a transferable Tight-Binding-Model"*.
  Supervisor: Prof. Dr. Stefan Blügel
- **Ph.D. thesis committee member / examiner (POSTECH)**,
  Seung-Gyo Jeong, *"Topological defects in quasi one dimensional charge density wave"*.
  Supervisor: Prof. Tae-Whan Kim

Short Term Visits

- **Aug. 8 2022 ∼ Aug. 31 2022**,
  School of Computational Sciences, Korea Institute for Advanced Study (KIAS), Seoul, Korea,
  Host: Prof. Young-Woo Son
- **Jun. 1 2018 ∼ Nov. 30 2018**,
  Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich, Jülich, Germany,
  Host: Prof. Stefan Blügel and Dr. Gustav Bihlmayer
- **Jul. 13 2015 ∼ Aug. 31 2015**,
  School of Computational Sciences, Korea Institute for Advanced Study (KIAS), Seoul, Korea,
  Host: Prof. Young-Woo Son
- **Feb. 26 ∼ Mar. 12 2015**,
  ICQM, Peking University, Beijing, China,
  Host: Prof. Ji Feng
- **Jan. 15 2015 ∼ Jun. 30 2015: Visiting student**,
  ICQD/HFNL, University of Science and Technology of China, Hefei, China,
  Host: Prof. Zhenyu Zhang
- **Jan. 15 2013 ∼ Jan. 27 2013**,
  ICQD/HFNL, University of Science and Technology of China, Hefei, China,
  Host: Prof. Changgan Zeng

- **Jul. 1 2011 ∼ Sep. 30 2011: Visiting student**,
  Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich, Germany,
  Host: Prof. Stefan Blügel
- **Dec. 1 2010 ∼ Feb. 14 2011: Visiting student**,
  Theory Department, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany,
  Host: Prof. Matthias Scheffler

Honors & Awards

- *Humboldt Research Fellowship for Postdoctoral Researchers*
  Alexander von Humboldt-Stiftung, 2020-2022
- *KIAS Academic Research Award*
  Korea Institute for Advanced Study, September 20 2018
- *TJ Park (Cheong-Am) Science Fellowship*
  POSCO TJ Park Foundation, 2018-2019
- *Outstanding PhD Dissertation Award*
  Hanyang University, August 21 2015
- *Outstanding Paper Award*
  Research Institute for Natural Sciences, Hanyang University, February 2015
- *Selected by the JSPS to participate in the "6th HOPE Meeting with Nobel Laureates"*
  Japan Society for the Promotion of Science (JSPS), March 11-15 2014 (Tokyo, Japan)
- *Best Presentation Award (Oral)*
  KPS Spring Meeting, The Korean Physical Society, Spring 26 2013
- *Hanyang Science and Technology Scholarship*
  Hanyang University, Spring 2011 - Fall 2012
- *DAAD-NRF Summer Institute Program (Scholarship & travel grant)*
  German Academic Exchange Service (Germany) and National Research Foundation (Korea), July-September 2011
- *Academic Excellence Scholarship*
  Hanyang University, Spring 2007

Research Grants

- *FZJ-NST Bilateral Cooperation Programme*
  Tight-binding Hamiltonian parameterizations using artificial intelligence
  Forschungszentrum Jülich (Germany) & National Research Council of Science and Technology (Korea), 2022 (Research fund: 50,000 EUR)
- *Humboldt Research Fellowship*
  The role of strain and interlayer interaction in the layered higher-order topological insulators: Multi-scale numerical simulations
  Alexander von Humboldt-Stiftung, 2020-2022 (Fellowship: 64,080 EUR)
- *Cheong-Am Science Fellowship*
  A study on the novel properties of low-dimensional crystalline matter
  POSCO TJ Park Foundation, 2018-2019 (Research fund: 70M KRW ∼ 57000 USD)

Computational skills

- **First-principles / quantum-chemistry codes:** FLEUR, VASP, FHI-aims, WIEN2k, AMS, Gaussian 16, ORCA
- **Programming:** Fortran, C, Python, Matlab/Octave, Shell (bash)

- **AI/ML & LLM stack (Python):** scikit-learn; PyTorch; gym (RL); langchain/langgraph (LLM app / agentic workflow prototyping)
- **Operating systems:** macOS, Linux, Windows
- **Open-source code development (selected):**
  - ***TBFIT*** (Fortran): Slater–Koster tight-binding parameter fitting toolkit. **Open-source impact (as of 2026): 33 stars / 16 forks** (github.com/Infant83/TBFIT)
  - ***VASPBERRY*** (Fortran): Berry curvature / Chern number post-processing for VASP `WAVECAR`. **Open-source impact (as of 2026): 77 stars / 29 forks; repository-linked PRB (2016) and PRL (2022) papers (150+ citations).** (github.com/Infant83/VASPBERRY)
  - ***VASPBAUM*** (Fortran): Band-unfolding machinery for VASP `WAVECAR` (k-projection), with optional circular dichroism. **Open-source impact (as of 2026): 7 stars / 3 forks**; maintained as a reusable post-processing pipeline. (github.com/Infant83/VASPBAUM)
  - *GitHub Arctic Code Vault Contributor (2020).*
- Course Certificates
  - **Post Graduate Program in Artificial Intelligence & Machine Learning**,
    Certified by Caltech Center for Technology and Management Education (CTME), May 05 2025, Simplilearn
  - **Quantum Programming Core**,
    Certificate of Course Completion: Quantum Programming Core, Aug. 15 2025, D-Wave

Brief account of my research topics

Research Interests (keywords): Density functional theory and beyond (vdW interactions, hybrid functionals, RPA, GW); electronic structure and quantum phenomena in low-dimensional systems; spin–orbit coupling and topological materials; quantum magnetism; AI/ML for materials discovery; quantum computing for optimization and molecular design.

My research focuses on computational materials science, with a core emphasis on **molecular/materials design using first-principles and quantum-chemical simulations**, and on **AI/ML workflows** that translate simulation outputs into data-driven screening and inverse-design strategies. I bring a strong background in condensed-matter theory and electronic-structure methods, developed through studies of graphene, 2D transition-metal dichalcogenides, topological materials, and surface/adsorption systems, where I produced mechanistic insights into structure-property relationships, magnetism, and electronic/topological properties. I have published **30+ peer-reviewed papers**, including in **Physical Review Letters / Physical Review B / Physical Review Materials**, ACS journals, and **Nature Portfolio journals** (e.g., *Scientific Reports*; *npj Computational Materials*), and have presented at major international conferences.

During my postdoctoral work, I incorporated **global optimization** into model development, including robust parameterization of **tight-binding Hamiltonians** for electronic/topological properties to enable multi-scale simulations. This experience shaped my approach to building reliable and transferable computational workflows that couple physics-based models with modern optimization and learning techniques, while maintaining interpretability and reproducibility.

In recent years, I have expanded my work toward **OLED-relevant molecular/materials design and mechanism analysis** in an industrial R&D environment. At LG Display, I apply quantum-chemical/DFT simulations and ML-enabled workflows to connect **structure–property relationships** to **emission and stability**, and to support data-driven material screening and design decisions. This includes developing ML strategies for **inverse design of blue TADF emitters**, trained on excited-state properties derived from DFT calculations (SID Display Week submission).

In parallel, I am pursuing a forward-looking agenda on **hybrid quantum–classical approaches** for materials discovery. My current focus is on **problem framing and feasibility analysis**—for example, reformulating OLED-relevant quantum-chemical objectives into optimization forms compatible with quantum optimization paradigms (e.g., QUBO-style formulations)—and on **workflow prototyping** that can later be evaluated in scoped pilot projects. This direction is an ongoing effort and should be interpreted as preparation for future execution, rather than completed QC outcomes.

Going forward, my goal is to build an **OLED-targeted materials discovery pipeline** that unifies (i) state-of-the-art quantum chemistry for property prediction, (ii) AI/ML workflows for data-efficient modeling and active learning, and (iii) inverse design supported by **generative AI** and, where appropriate, **quantum optimization**, aligned with industrial strategies that aim to accelerate discovery-to-deployment for next-generation OLED materials.

Peer-Reviewed Publications

Papers submitted / in preparation

1. **Hyun-Jung Kim**, Irene Aguilera, Christoph Friedrich, Gustav Bihlmayer, and Stefan Blügel, *Transferable empirical tight-binding model for Bi bulk and thin films*, ***in preparation***.

2. **Hyun-Jung Kim**, Seoung-Hun Kang, Hyungjun Lee, Gyu Hyung Kim, and Young-Woo Son, *Nodal fermion in the surface states of Bi adsorbed (110) surface of group-IV semiconductors*, ***in preparation***.

Published papers in *American Physical Society* journals

• Physical Review Letters

3. Sun-Woo Kim, **Hyun-Jung Kim**†, Sangmo Cheon†, and Tae-Hwan Kim†, *Circular Dichroism of Emergent Chiral Stacking Orders in Quasi-One-Dimensional Charge Density Waves*, ***Phys. Rev. Lett.*** 128, 046401 (2022) [† **corresponding author**]

4. Shuyuan Liu, Chongze Wang, Lianglinang Liu, Jin-Ho Choi, **Hyun-Jung Kim**, Yu Jia, Chul Hong Park, and Jun-Hyung Cho, *Ferromagnetic Weyl Fermions in Two-Dimensional Layered Electride* Gd_2C, ***Phys. Rev. Lett.*** 125, 187203 (2020).

5. Sun-Woo Kim*, Yoon-Gu Kang*, **Hyun-Jung Kim***, and Jun-Hyung Cho, *Comment on "Quasi-One-Dimensional Metal-Insulator Transitions in Compound Semiconductor Surfaces"*, ***Phys. Rev. Lett.*** 118, 239601 (2017). **[*contributed equally]**

6. Sun-Woo Kim, Chen Liu, **Hyun-Jung Kim**, Jun-Ho Lee, Yongxin Yao, Kai-Ming Ho, and Jun-Hyung Cho, *Nature of the Insulating Ground State of 5d Post-Perovskite* $CaIrO_3$, ***Phys. Rev. Lett.*** 115, 096401 (2015).

7. Hui Zhang*****, Fangfei Ming*****, **Hyun-Jung Kim***, Hongbin Zhu, Changgan Zeng, Qiang Zhang, Hanno Weitering, Xudong Xiao, Jun-Hyung Cho, and Zhenyu Zhang, *Stabilization and Manipulation of Electronically Phase-Separated Ground States in Defective Indium Atom Wires on Silicon*, ***Phys. Rev. Lett.*** 113, 196802 (2014). **[*contributed equally]**
→***Selected as outstanding research achievement*** (National Research Foundation, Grant No. 2014M2B2A9032247)

8. Jun-Ho Lee, **Hyun-Jung Kim**, and Jun-Hyung Cho, *Ferrimagnetic Slater Insulator Phase of the Sn/Ge(111) Surface*, ***Phys. Rev. Lett.*** 111, 106403 (2013).

9. **Hyun-Jung Kim** and Jun-Hyung Cho, *Driving Force of Phase Transition in Indium Nanowires on Si(111)*, ***Phys. Rev. Lett.*** 110, 116801 (2013).

• **Physical Review B: Rapid Communication**

10. Sun-Woo Kim, **Hyun-Jung Kim**†, Sangmo Cheon†, and Tae-Hwan Kim†, *Two-dimensional chiral stacking orders in quasi-one-dimensional charge density waves*, ***Phys. Rev. B (Rap. Comm.)*** 102, 121408 (2020). [† **corresponding author**]

11. **Hyun-Jung Kim**, Seoung-Hun Kang, Ikutaro Hamada, and Young-Woo Son, *Origins of the structural phase transitions in $MoTe_2$ and WTe_2*, ***Phys. Rev. B (Rap. Comm.)*** 95, 180101 (2017).

12. **Hyun-Jung Kim**, Chaokai Li, Feng Ji, Jun-Hyung Cho, and Zhenyu Zhang, *Competing magnetic orderings and tunable topological states in two-dimensional hexagonal organometallic lattices*, ***Phys. Rev. B (Rap. Comm.)*** 93, 041404 (2016).

→***Selected as outstanding research achievement*** (Korea Insitute for Advanced Study)

13. **Hyun-Jung Kim**, Alexandre Tkatchenko, Jun-Hyung Cho, and Matthias Scheffler, *Benzene adsorbed on Si(001): The role of electron correlation and finite temperature*, ***Phys. Rev. B (Rap. Comm.)*** 85, 041403 (2012).

14. **Hyun-Jung Kim**, Sangchul Oh, Ki-Seok Kim, Zhenyu Zhang, and Jun-Hyung Cho, *Length- and parity-dependent electronic states in one-dimensional carbon atomic chains on C(111)*, ***Phys. Rev. B (Rap. Comm.)*** 82, 041401 (2010). → ***Selected in "Virtual Journal of Nanoscale Science & Technology", Vol. 22, July 19 (2010).***

• **Physical Review B**

15. Seoung-Hun Kang, Sangjun Jeon, **Hyun-Jung Kim**, Wonhee Ko, Suyeon Cho, Se Hwang Kang, Heejun Yang, Hyo Won Kim, and Young-Woo Son, *Reshaped Weyl fermionic dispersions driven by Coulomb interactions in $MoTe_2$*, ***Phys. Rev. B*** 105, 045143 (2022).

16. Sang-Min Jeong*, Seho Yi*, **Hyun-Jung Kim***, Gustav Bihlmayer, and Jun-Hyung Cho, *Competing edge structures of Sb and Bi bilayers generated by trivial and nontrivial band topologies*, ***Phys. Rev. B*** 96, 075416 (2018). **[*contributed equally]**

17. Sun-Woo Kim, Hyun Jung, **Hyun-Jung Kim**, Jin-Ho Choi, Su-Huai Wei, and Jun-Hyung Cho, *Microscopic mechanism of the tunable band gap in potassium-doped few-layer black phosphorus*, ***Phys. Rev. B*** 96, 075416 (2017).

18. Xiao-Yan Ren, **Hyun-Jung Kim**, Seho Yi, Yu Jia, and Jun-Hyung Cho, *Spin-orbit coupling effects on the stability of two competing structures in Pb/Si(111) and Pb/Ge(111)*, ***Phys. Rev. B*** 94, 075436 (2016).

19. **Hyun-Jung Kim** and Jun-Hyung Cho, *Giant spin-orbit-induced spin splitting in Bi chains on GaAs(110)*, ***Phys. Rev. B*** 92, 085303 (2015).

20. Sun-Woo Kim, **Hyun-Jung Kim**, Jin-Ho Choi, Ralph H. Scheicher, and Jun-Hyung Cho, *Contrasting interedge superexchange interactions of graphene nanoribbons embedded in h-BN and graphane*, ***Phys. Rev. B*** 92, 035443 (2015).

21. Sun-Woo Kim, **Hyun-Jung Kim**, Fangfei Ming, Yu Jia, Changgan Zeng, Jun-Hyung Cho, and Zheunyu Zhang, *Equivalence of electronic and mechanical stresses in structural phase stabilization: A case study of indium wires on Si(111)*, ***Phys. Rev. B*** 91, 174434 (2015).

22. **Hyun-Jung Kim** and Jun-Hyung Cho, *Fluorine-induced local magnetic moment in graphene: A hybrid DFT study*, ***Phys. Rev. B*** 87, 174435 (2013).

23. **Hyun-Jung Kim**, Sangchul Oh, and Jun-Hyung Cho, *Peierls instability and ferrimagnetic ordering of quasi-one-dimensional carbon chains generated in H-passivated graphene*, ***Phys. Rev. B*** 83, 235408 (2011).

• **Physical Review Materials**

24. Bharti Parashar, Lars Rathmann, **Hyun-Jung Kim**, Iulia Cojocariu, Aaron Bostwick, Chris Jozwiak, Eli Rotenberg, José Avila, Pavel Dudin, Vitaliy Feyer, Christoph Stampfer, Bernd Beschoten, Gustav Bihlmayer, Claus M. Schneider, and Lukasz Plucinski, *Photoemission study of twisted monolayers and bilayers on WSe_2 on graphite substrates*, ***Phys. Rev. Mater.*** 7, 044004 (2023).

25. Irene Aguilera, **Hyun-Jung Kim**, Christoph Friedrich, Gustav Bihlmayer, and Stefan Blügel, *Z_2 topology of bismuth*, ***Phys. Rev. Mater.*** 5, L091201 (2021).

Published papers in *American Chemical Society* journals

26. Hyo Won Kim*, Seoung-Hun Kang*, **Hyun-Jung Kim***, Kisung Chae, Suyeon Cho, Wonhee Ko, Sangjun Jeon, Se Hwang Kang, Heejun Yang, Sung Wng Kim, Seongjun Park, Sungwoo Hwang, Young-Kyun Kwon, Young-Woo Son, *Symmetry Dictated Grain Boundary State in a Two-dimensional Topological Insulator*, ***Nano. Lett.*** 20, 5837 (2020) **[*contributed equally]**

27. Jun-Ho Lee, Yun-Ki Choi, **Hyun-Jung Kim**, Ralph H. Scheicher, and Jun-Hyung Cho, *Physisorption of DNA Nucleobases on h-BN and Graphene: vdW-Corrected DFT Calculations*, ***J. Phys. Chem. C*** 117, 13435 (2013).

28. **Hyun-Jung Kim**, Sangchul Oh, Changgan Zeng, and Jun-Hyung Cho, *Peierls Instability and Spin Orderings of Ultranarrow Graphene Nanoribbons in Graphane*, ***J. Phys. Chem. C*** 116, 13795 (2012).

Published papers in other journals

29. **Hyun-Jung Kim***, Junho Lee*, Yeol Kyo Choi, Taeyang Lee, Joong-Hwan Yang, Sung Moon Ko, Dae-Woong Jeong, Sehui Han, Jeongguk Min, Ji-Ho Baek, Seok-Woo Lee, Joon-Young Yang, Soo-Young Yoon, *85-3: Machine Learning Strategy Towards Inverse Design of Blue TADF Emitter: Training Excited State Properties Based on Density Functional Theory Calculations*, ***SID Symposium Digest of Technical Papers*** 55, 1183 (2024). **[*contributed equally]**

30. Yu Dai, Wenjiang Zhou, **Hyun-Jung Kim**, Qichen Song, Xin Qian, Te-Huan Liu, and Ronggui Yang, *Simultaneous enhancement in electrical conductivity and Seebeck coefficient by single- to double-valley transition in a Dirac-like band*, ***npj Comput. Mater.*** 8, 234 (2022).

31. Huije Ryu, Yangjin Lee, **Hyun-Jung Kim**, Seoung-Hun Kang, Yoongu Kang, Kangwon Kim, Jungcheol Kim, Blanka E. Janicek, Kenji Watanabe, Takashi Taniguchi, Pinshane Y. Huang, Hyeonsik Cheong, In-Ho Jung, Kwanpyo Kim, Young-Woo Son, and Gwan-Hyoung Lee, *Anomalous Dimensionality-driven Phase Transition of $MoTe_2$ in van der Waals Heterostructure*, ***Adv. Func. Mater.*** 31, 2107376 (2021).

32. Seho Yi, Jin-Ho Choi, **Hyun-Jung Kim**, Chul Hong Park, and Jun-Hyung Cho, *Contrasting diffusion behaviors of O and F atoms on graphene and within bilayer graphene*, ***Phys. Chem. Chem. Phys.*** 19, 9107-9112 (2017).

33. Xiao-Yan Ren, **Hyun-Jung Kim**, Chun-Yao Niu, Yu Jia, Jun-Hyung Cho, *Origin of Symmetric Dimer Images of Si(001) Observed in Low-Temperature STM*, ***Sci. Rep.*** 6, 27868 (2016).

34. **Hyun-Jung Kim**, Jun-Ho Lee, and Jun-Hyung Cho, *Antiferromagnetic Slater Insulator Phase of Na_2IrO_3*, ***Sci. Rep.*** 4, 5253 (2014).
→***Selected in Outstanding Paper Award*** (Research Institute for Natural Sciences, Hanyang University, 2015)

35. Sun-Woo Kim, Jun-Ho Lee, **Hyun-Jung Kim**, and Jun-Hyung Cho, *Contribution of van der Waals interactions to the adsorption energy of C2H2, C2H4, and C6H6 on Si(100)*, ***Chem. Phys. Lett*** 557, 159 (2013).

36. **Hyun-Jung Kim**, Xingyong Wang, Jing Ma, and Jun-Hyung Cho, *A density-functional-theory study of biradicals from benzene to hexacene*, ***Chem. Phys. Lett.*** 516, 141 (2011).

Talks and Presentations

• Contributed Talks

1. *Machine Learning Strategy Towards Inverse Design of Blue TADF Emitter: Training Excited State Properties Based on Density Functional Theory Calculations*
SID Display Week 2024 Symposium, San Jose, USA, May 2024.

2. *An open-source software package for Slater-Koster tight-binding parameterization and calculation*
Korean Physical Society Spring Meeting, Korea, April 2019.

3. *Weyl fermion in the surface states of Bi adsorbed Si(110) surface with nonsymmorphic lattice*
Korean Physical Society Spring Meeting, Korea, April 2018.

4. *Weyl fermion on reconstructed surface of Bi/Si(110) with non-symmorphic lattice symmetry*
APS March Meeting, USA (L.A.), March 2018.

5. *Origins of Structural Phase Transition in bulk $MoTe_2$ and WTe_2*
Korean Physical Society Spring Meeting, Korea, April 2017.

6. *A van der Waals density functional study of structural phase transition in bulk $MoTe_2$ and WTe_2*
APS March Meeting, USA (New Orleans), March 2017.

7. *A van der Waals density functional study of interlayer interaction and phase stability in layered transition metal dichalcogenides MTe_2 (M=Mo, W)*
Korean Physical Society Fall Meeting, Korea, October 2016.

8. *Spin-valley coupling and topological phase transition in antiferromagnetic 2D organometallic thin film*
33rd International Conference on the Physics of Semiconductors, China (Beijing), July-August 2016.

9. *Electric field induced quantum anomalous Hall effect in two-dimensional antiferromagnetic triphenyllead lattice*
APS March Meeting, USA (Baltimore), March 2016.

10. *Electric field induced topological phase transition in 2D organometallic lattice*
The 15th International Conference on the Formation of Semiconductor Interfaces, Japan (Hiroshima), November 2015.

11. *Giant spin-orbit-induced spin splitting in Bi zigzag chains on GaAs(110)*
Korean Physical Society Fall Meeting, Korea, October 2015.

12. *Structural phase transition in nanowire controlled by strain and electric field*
Korean Physical Society Spring Meeting, Korea, April 2014.

13. *Structural and electronic properties of indium nanowires on Si(111)*
The 10th Workshop on Surface Nano-Science, Korea, February 2014.

14. *Fluorine-induced local magnetic moment in graphene: A hybrid DFT study*
45th Annual Conference of the Korean Vacuum Society, Korea, August 2013.

15. *Driving Force of Phase Transition in Indium Nanowires on Si(111)*
The 14th International Conference on the Formation of Semiconductor Interfaces, Korea, July 2013.

16. *Robustness of Topological Edge States Against Peierls Distortion and Reconstruction*
Korean Physical Society Spring Meeting, Korea, April 2013.

17. *Driving Force of Phase Transition in Indium Nanowires on Si(111)* ****Best Presentation Award winner***
Korean Physical Society Spring Meeting, Korea, April 2013.

18. *Robustness of Topological Edge States Against Peierls Distortion and Reconstruction*
The 9th Asian Workshop on Surface Nano-Science, Korea, February 2013.

19. *Peierls instability and spin orderings of ultranarrow graphene nanoribbons in graphane*
Korean Physical Society Spring Meeting, Korea, April 2012.

20. *Peierls instability and spin orderings in graphane*
42th Annual Conference of the Korean Vacuum Society, Korea, February 2012.

21. *Benzene Adsorbed on Si(001): The Role of Electron Correlation and Finite Temperature*
The 8th Asian Workshop on Surface Nano-Science, Korea, January 2012.

22. *The Structure of Benzene on Si(001) at Zero and Finite Temperatures: Electronic Correlation and Vibrational Effects*
Korean Physical Society Fall Meeting, Korea, October 2011.

23. *Electron correlation effect in the adsorption of benzene on Si(100) within van der Waals density functional scheme and random phase approximation*
Korean Physical Society Spring Meeting, Korea, April 2011.

24. *Length- and parity-dependent electronic states in one-dimensional carbon atomic chains on C(111)*
39th Annual Conference of the Korean Vacuum Society, Korea, August 2010.

• Non-invited Talks & Departmental Seminar

1. *Introduction to Quantum Computing and Perspectives*
"DX Tech Seminar", Hosted by AI/Big Data Division, LG Display, Korea, 21 February 2025.

2. *GOETHE: Global Optimization toolkit for Empirical Tight-binding model Hamiltonian Evaluation*
"Laboratory Seminar", Hosted by Joong-Whan Yang, LG Display, Korea, 28 September 2022.

3. *Tight-binding Hamiltonian parameterization using machine learning*
"Group seminar", Hosted by Prof. Dr. Peter Kratzer, Universität Duisburg-Essen, Duisburg, Germany, 09 June 2022.

4. *Circular Dichroism of Emergent Chirality in Quasi-One-Dimensional Charge Density Waves*
"Quantum Theory of Materials seminar", Hosted by Prof. Dr. Stefan Blügel, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany, 09 March 2022.

5. *Electronic properties of twisted WSe_2 bilayers and WSe_2 single layer on graphene*
Hosted by Prof. Dr. Young-Woo Son, Computational Sciences, Korea Institute for Advanced Study, Korea, 17 February 2022.

6. *Tight binding approximations and its application to bismuth and transition metal dichalcogenides*
"Laboratory Seminar", Hosted by Prof. Dr. Jun-Hyung Cho, Electronic Structure Theory Group, Department of Physics, Hanyang University, Korea, 13 February 2022.

7. *Two-dimensional chiral stacking orders in quasi-one-dimensional charge density waves*
"Quantum Theory of Materials seminar", Hosted by Prof. Dr. Stefan Blügel, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany, 02 December 2020.

8. *Computational approaches on structural, electronic, and topological properties in low dimensional systems*
Department of Physics Symposium 2019, Department of Physics, Hanyang University, 20 September 2019.

9. *TBFIT: An open-source software package for Slater-Koster tight-binding parameter fitting*
"Quantum Theory of Materials seminar", Hosted by Dr. Gustav Bihlmayer, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany, 28 November 2018.

10. *Weyl fermion in the surface states of Bi adsorbed Si(110) surface*
"Quantum Theory of Materials seminar", Hosted by Dr. Gustav Bihlmayer, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany, 20 June 2018.

11. *Emergence of massless Weyl fermion in two dimensional system*
2018 Computational Sciences Workshop, Korea Institute for Advanced Study (KIAS), Korea, 11 May 2018.

12. *Structural, electronic, and topological phase transitions in low dimensional systems*
Hosted by Prof. Young-Kyu Han, Department of energy and materials engineering, Dongguk University, Korea, 27 September 2017.

13. *Spin-valley Coupling and Tunable Topological States in Two-dimensional Antiferromagnetic Triphenyl-Lead Lattices*
Hosted by Prof. Noejung Park, Department of Physics, Ulsan National Institute of Science and Technology (UNIST), Korea, 19 October 2015.

14. *A first-principles density functional theory study of tunable topological states in two-dimensional antiferromagnetic triphenyl-lead lattices*
2015 Computational Sciences Workshop, Korea Institute for Advanced Study (KIAS), Korea, 16 October 2015.

15. *Giant Rashba type Spin Splitting in 1-D Bi Chains on GaAs(110)*
Hosted by Dr. Kun Woo Kim, Journal Club, Korea Institute for Advanced Study (KIAS), Korea, 15 July 2015.

16. *The structural/electronic stability in valley polarized AFM state in 2D metal organic framework*
Hosted by Prof. Zhenyu Zhang, ICQD Brainstorming session, ICQD, University of Science and Technology of China, China, 20 March 2015.

17. *Electronic structure in one-dimensional systems: Graphene nanoribbon in graphene, In/Si nanoarray, Bi(111) nanoribbon*
Hosted by Prof. Changgan Zeng, ICQD Brainstorming session, ICQD, University of Science and Technology of China, China, 24 January 2013.

18. *Benzene Adsorbed on Si(001): The Role of Electron Correlation and Finite Temperature*
Departmental workshop, Department of Physics 2011 Symposium , Hanyang University, Korea, 18 November 2011.

19. *Competing Charge and Spin Orderings of One-dimensional C-chains*
    Hosted by Prof. Stefan Blügel, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany, 27 July 2011.

20. *A first-principles study of Benzene/Si(100): Role of van der Waals interactions*
    Hosted by Prof. Matthias Scheffler, Coffee Talk, Theory Department, Fritz-Haber-Institut, Germany, 7 February 2011.

• Poster Presentations

1. *The role of strain and interlayer interaction in the layered higher-order topological insulators: Multi-scale numerical simulations*
   Virtual Network Meeting of the Alexander von Humboldt Foundation (Virtual Venue), Nov. 18-19 2020.

2. *TBFIT: An open-source software package for Slater-Koster tight-binding parameter fitting*
   Workshop on Computational Physics and Materials Science: Total Energy and Force Method, Spain (Donostia-San Sebastian), Jan. 08 2020.

3. *Six-nearest-neighbor parameterized Slater-Koster tight-binding model for bismuth*
   The 22nd Asian Workshop on First-Principles Electronic Structure Calculations, Japan (Osaka), Oct. 27 2019.

4. *Six-nearest-neighbor parameterized Slater-Koster tight-binding model for Bi*
   11th Recent Progress in Graphene & 2D Materials, Japan (Matsue), Oct. 7∼10 2019.

5. *TBFIT: An open-source software package for Slater-Koster tight-binding parameter fitting*
   Automated Interactive Infrastructure and Database for Computational Science, Switzerland (EPFL, Lausanne), May. 21∼24 2019.

6. *Nodal fermion in the surface states of Bi adsorbed semiconductor surface*
   The 56th Winter Annual Conference of the Korean Vacuum Society, Korea (Hongcheon), Feb. 18∼20 2019.

7. *Adsorption structure of Bi adatom induced Si(110)-(3×2) surface*
   The 54th Winter Annual Conference of the Korean Vacuum Society, Korea (Hoengseong), Feb. 7∼9 2018.

8. *Intertwined structural and electronic phase transition in layered transition metal dichalcogenides: $MoTe_2$ and WTe_2*
   The 20th Asian Workshop on First-Principles Electronic Structure Calculations, China (Nanjing), Oct. 31∼Nov. 1 2017.

9. *Contrasting structural and electrical phase transition behaviors of layered transition metal dichalcogenides $MoTe_2$ and WTe_2*
   2017 Recent Progress in Graphene & Two-Dimensional Materials Research, Singapore, Sep. 19∼22 2017.

10. *Interlayer interaction and phase stability in bulk MoTe2 and WTe2: A van der Waals density functional study*
    The 19th Asian Workshop on First-Principles Electronic Structure Calculations, Taiwan (Hsinchu), Oct. 31∼ Nov. 2 (2016).

11. *Electric field induced quantum anomalous Hall effect in spin-valley coupled 2D triphenyl-lead monolayer*
    The 1st USTC-FHI workshop on the Frontiers of Advanced Electronic Structure Methods, China (Hefei), June 2016.

12. *Magnetic ordering and topological phase transition in 2D organometallic thin film: $Pb_2[C_3H_5]_3$ lattice*
The 18th Asian Workshop on First-Principles Electronic Structure Calculations, Japan (Tokyo), November 2015.

13. *Tunable Topological States in Hexagonal Triphenyl-lead Lattice*
7th International Conference on Recent Progress in Graphene (and Two-dimensional Materials) Research, Australia (Victoria), October 2015.

14. *Electronic properties in 2D hexagonal triphenyl-lead lattice and topological phase transition via applied E-field*
Korea Supercomputing Conference 2015, Korea, October 2015.

15. *Strain and electric-field controlled phase transition in indium atom wires on silicon*
The 1st International Conference & Exhibition for Nanopia, Korea, November 2014.

16. *Strain and Electric Field Effect on Phase Transition in Indium Atomic Wire on Silicon Surface*
IPAM GSS2014 :"Electronic Structure Theory for Materials and (Bio)molecules", USA (L.A.), July-August 2014.

17. *Metal-Insulator Phase Transition in Indium Nanowires on Si(111) surface*
The 6th HOPE Meeting (Japan Society for the Promotion of Science), Japan (Tokyo),March 2014.

18. *Effects of Self-Interaction Correction and Spin-Orbit Coupling on the Insulating Phase of Na_2IrO_3*
2014 Quantum Materials Symposium - in conjunction with 14th Korea-Japan-Taiwan Workshop on SCES, Korea, February 2014.

19. *Role of strain and electric field in phase transition of indium nanowire on Si(111)*
Korean Physical Society Fall Meeting, Korea, October 2013.

20. *Influence of geometry on the edge states of Bi Nanoribbons*
The 19th International Conference on Magnetsim, Korea, July 2012.

21. *Influence of spin delocalization on the singlet-triplet gap of diradicals generated in polyacenes: Density-functional theory calculations*
Korean Physical Society Fall Meeting, Korea, October 2010.