Ji-Sang Park, Ph. D.

Department of Nano Engineering Sungkyunkwan University 2066, Seobu-ro, Jangan-gu, Suwon-si, Gyeonggi-do Republic of Korea Email: <u>jisangpark@skku.edu</u>

PERSONAL INFORMATION

Citizenship Republic of Korea

EDUCATION

- 2007-2013 Ph.D., Physics, **KAIST**, Daejeon, Republic of Korea Dissertation: First-principles study of defects and impurities in semiconductor nanowires and nitrides Supervisor: Prof. Kee Joo Chang <u>kchang@kaist.ac.kr</u>
- 2003-2007 Bachelor of Science, Double major in Mathematics and Physics, **KAIST**, Daejeon, Republic of Korea

RESEARCH EXPERIENCE

2022-present	Assistant Professor, SKKU Advanced Institute of Nano Technology (SAINT) & Department of Nano Engineering, Sungkyunkwan University
2019-2022	Assistant Professor, Department of Physics, Kyungpook National University
2018-2019	Royal Society - Shooter International Fellow , Imperial College London (ICL), London UK
2017-2018	Research Associate, Imperial College London (ICL), London, UK Supervisor: Prof. Aron Walsh <u>a.walsh@imperial.ac.uk</u>
2016-2017	Postdoctoral Researcher, Argonne National Laboratory (ANL), Lemont, IL, USA Supervisor: Dr. Maria K. Y. Chan <u>mchan@anl.gov</u>
2013-2016	Postdoctoral Researcher, National Renewable Energy Laboratory (NREL), Golden, CO, USA Supervisor: Prof. Su-Huai Wei <u>suhuaiwei@csrc.ac.cn</u>
2009-2013	Technical Research Personnel for Military service, KAIST , Daejeon, Republic of Korea
2007-2013	Research Assistant, KAIST , Daejeon, Republic of Korea Supervisor: Prof. Kee Joo Chang <u>kchang@kaist.ac.kr</u>

SELECTED PUBLICATIONS

- J.-S. Park, et al., Point defect engineering in thin-film solar cells, <u>Nature Reviews</u> <u>Materials</u> 3, 194–210 (2018).
- Ji-Sang Park and Aron Walsh, Embrace your defects, Nature Energy 4, 95–96 (2019).
- S. Y. Park, <u>J.-S. Park (co-first)</u>, B. J. Kim, H. Lee, A. Walsh, K. Zhu, D. H. Kim, and H. S. Jung, Sustainable Lead Management in Halide Perovskite Solar Cells, Nature Sustainability 3, 1044–1051 (2020).
- J.-S. Park, et al., *Hexagonal Stacking Faults Act as Hole-Blocking Layers in Lead Halide Perovskites*, ACS Energy Lett. 5, 2231–2233 (2020).
- J.-S. Park, et al., Accumulation of Deep Traps at Grain Boundaries in Halide Perovskites, ACS Energy Lett. 4, 1321 (2019).
- J.-S. Park and A. Walsh, *Modelling Grain Boundaries in Polycrystalline Halide Perovskite Solar Cells*, Annu. Rev. Condens. Matter Phys. 12, 95-109 (2021).
- A. Walsh and <u>J.-S. Park</u>, *The Holey Grail of Transparent Electronics*, Matter 3, 604-606 (2020).

AWARDS

- 1. Outstanding Reviewer for Journal of Physics: Condensed Matter in 2019
- 2. First Prize (Poster), The Solid State Chemistry Group Christmas Meeting, 18th December 2018, London, United Kingdom
- 3. <u>The Young Physicist Award</u>, The Korean Physical Society (KPS), October 24, 2018, Changwon, Republic of Korea
- 4. <u>Royal Society Shooter International Fellowship</u>, The Royal Society, October 11, 2017, London, United Kingdom
- 5. <u>The 3rd Distinguished Dissertation Award of This Year (Physics)</u>, The Korean Academy of Science and Technology (KAST), November 29, 2013, Seoul, Republic of Korea
- 6. Best Poster Awards at the Korean Physical Society Spring Meeting, November 1, 2013, Changwon, Republic of Korea
- 7. Best Presentation Awards, The Korean Physical Society Spring Meeting, April 26, 2013, Daejeon, Republic of Korea
- 8. Best Poster Award (Bronze), The 5th BK21 Young Physicists Workshop, January 13, 2012, Daejeon, Republic of Korea
- 9. Best Presentation Awards, The Korean Physical Society Spring Meeting, April 15, 2011, Daejeon, Republic of Korea

- 10. Best Poster Award (Bronze) at The 4th BK21 Young Physicists Workshop, January, 21, 2011, Pohang, Republic of Korea
- 11. Best Poster Award at The 6th KIAS Electronic Structure Calculation Workshop, June 21-22, 2010, Seoul, Republic of Korea
- 12. Student Poster Awards at International Conference on Core Research and Engineering Science of Advanced Materials, June 3, 2010, Osaka, Japan
- 13. Best Paper Award (Oral presentation) at The 3rd BK21 Young Physicists Workshop, January 15, 2010, Seoul, Korea
- 14. Outstanding Teaching Assistant Awards, Department of Physics, KAIST, for Advanced Solid State Physics I, September 7, 2009, Daejeon, Republic of Korea

FUNDING

- 2020-2023 : Principal Investigator (연구책임자), General Research Program (기본연구), National Research Foundation of Korea (Grant No. 2020R1F1A1053606)
- 2019-2022 : Co-researcher (공동연구원), Material Convergence Innovation Technology Development Program (소재융합혁신기술개발), National Research Foundation of Korea (Grant No. 2019M3D1A2104108)
- 2018-2019 : Principal Investigator (연구책임자), Royal Society Shooter International Fellowship, The Royal Society (Grant No. NF170826)

PROFESSIONAL ACTIVITIES

- Reviewer for 28 journals including Nature Materials, ACS Energy Letters, Nature Communications, Journal of Materials Chemistry A, Journal of Physical Chemistry Letters, Journal of Physics: Energy, Nanoscale, Applied Physics Letters.
- (2021) Guest Editor for JPhys Energy (Online ISSN 2515-7655), Focus on Grand Challenges in Halide Perovskites: Defects
- (2021) Section Editor of Symmetry (EISSN 2073-8994)
- Program Committee for The 12th International Conference on Advanced Materials and Devices (ICAMD 2021)

TEACHING EXPERIENCES

Sungkyunkwan University

• Introduction to Modeling and simulation (Fall 2022)

Kyungpook National University

- <u>Solid state physics</u> (Spring 2022)
- <u>Statistical Physics</u> (graduate) (Spring 2022)
- <u>Thermal Physics</u> (Spring 2021), <u>Statistical Physics</u> (Fall 2021)

- <u>Physics I</u> (Spring 2020, Spring 2021), <u>Physics II</u> (Fall 2019, Fall 2020, Fall 2021)
- Physics Lab. I (Spring 2020), Physics Lab. II (Fall 2020, Fall 2019)
- <u>Computational Simulation and Modeling</u> (graduate) (Fall 2020)
- Advanced Solid State Physics (graduate) (Spring 2020)
- <u>Selected Topics in Condensed Matter Physics</u> (graduate) (Fall 2019)

RESEARCH INTERESTS

- 1. Calculation of quantum materials by using first-principles DFT
- 2. Materials design based on efficient high-throughput calculations
- 3. Point defects ad extended defects (grain boundaries, dislocations) in semiconductors
- 4. Semiconductor devices including photovoltaics and light-emitting diodes

SUMMARY OF PUBLICATION

- Google Scholar Citations > 4000, h-index 28, i10-index 45
- https://scholar.google.com/citations?hl=en&user=ZCmm3y8AAAAJ

FULL PUBLICATION (corresponding authored)

- C. U. Lee, S. Ma, J. Ahn, J. Kyhm, J. Tan, H. Lee, G. Jang, Y. S. Park, J. Yun, J. Lee, J. Son, J.-S. Park, and J. Moon, Tailoring the Time-Averaged Structure for Polarization-Sensitive Chiral Perovskites, accepted for publication in J. Am. Chem. Soc.
- Boseong Kim, Youbin Song, and <u>Ji-Sang Park</u>, Comparison of Au nanocrystals predicted using the linear combination of atomic orbitals and plane waves, New Phys.: Sae Mulli 72, 558-563 (2022).
- Jeongjun Kim, Youbin Song, and Ji-Sang Park, Atomic structure and electronic structure of Si_{1-x}Ge_x and Al_xGa_{1-x}N: a density functional theory calculation, New Phys.: Sae Mulli 72, 481-486 (2022).
- Heejung Kong, Haechang Yang, Ji-Sang Park, Weon-Sik Chae, Hee Yeong Kim, Jucheol Park, Jong Hoon Lee, Seung Yo Choi, Miok Park, Hyeonwoo Kim, Youbin Song, Hyunwoong Park, Junyeob Yeo, Spatial Control of Oxygen Vacancy Concentration in Monoclinic WO3 Photoanodes for Enhanced Solar Water Splitting, Advanced Functional Materials (2022).
- 5. Kanghyeon Park, Byeong-Hyeon Jeong, and **Ji-Sang Park**, Search of chalcopyrite materials based on hybrid density functional theory calculation, Journal of Physics Communications 6(6) 065001 (2022).
- 6. Seok Lee, Youbin Song, and Ji-Sang Park, First-principles density functional theory calculation of bulk SnO2 and grain boundaries, 72(5) 336-341 (2022).
- 7. Ji-Sang Park, Stabilization and Self-Passivation of Grain Boundaries in Halide Perovskite by Rigid Body Translation, J. Phys. Chem. Lett. 13(20), 4628–4633 (2022).
- 8. Y. Song, S. Park, and <u>J.-S. Park</u>, Cost-effective calculation of defects in Si using hybrid density functional with downsampled reciprocal grids, Curr. Appl. Phys. 39, 51-55 (2022).

- Heejung Kong, Ji-Sang Park, Jong Hwa Kim, Suwon Hwang, and Junyeob Yeo, Hydrothermal Synthesis in Gap: Conformal Deposition of Textured Hematite Thin Films for Efficient Photoelectrochemical Water Splitting, ACS Applied Materials & Interfaces 14(14) 16515–16526 (2022).
- 10. Y. Song and J.-S. Park, Hybrid density functional theory calculation of orthorhombic CsPbI_{3-3x}Br_{3x} and CsPbBr_{3-3x}Cl_{3x}, Curr. Appl. Phys. 36, 93-96 (2022).
- S. H. Lee, K.-H. Kim, E. S. H. Kang, <u>J.-S. Park</u>, Effect of Distance Between Molecules on the Optoelectronic Property of PEDOT, New Phys.: Sae Mulli 71, 1004 (2021).
- Ji-Sang Park, Cost-Effective Hybrid Density Functional Theory Calculation of Three-Dimensional Band Structure and Search of Band Edge Positions, J. Phys. Chem. A 125, 8514–8518 (2021).
- Ji-Sang Park, Jina Jung, and Sangwook Lee, Cost-Effective High-Throughput Calculation Based on Hybrid Density Functional Theory: Application to Cubic, Double, and Vacancy-Ordered Halide Perovskites, J. Phys. Chem. Lett. 12, 7885–7891 (2021).
- 14. Zhenzhu Li, **Ji-Sang Park**, and Aron Walsh, Evolutionary exploration of polytypism in lead halide perovskites, **Chem. Sci.** 12, 12165 (2021).
- 15. Byeong-Hyeon Jeong, Minwoo Jeong, Youbin Song, Kanghyeon Park, and <u>Ji-Sang Park</u>, Screening of II-IV-V2 Materials for Photovoltaic Applications Based on Density Functional Theory Calculations, Crystals, 11, 883 (2021).
- B.-H. Jeong and J.-S. Park, Stability and electronic structure of stacking faults and polytypes in ZnSnN₂, ZnGeN₂, and ZnSiN₂, J. Korean Phys. Soc. 79, 309 (2021).
- 17. J.-S. Park and A. Walsh, *Modelling Grain Boundaries in Polycrystalline Halide Perovskite* Solar Cells, Annu. Rev. Condens. Matter Phys. 12, 95-109 (2021).
- **18.** <u>Ji-Sang Park</u>, Comparison study of exchange-correlation functionals on prediction of ground states and structural properties, Curr. Appl. Phys. 22, 61 (2021).
- 19. Kanghyeon Park, Byeong-Hyeon Jeong, Hui Yeor Lim, and <u>Ji-Sang Park</u>, *Effect of chemical substitution on polytypes and extended defects in chalcopyrites: a density functional theory study*, J. Appl. Phys. 129, 025703 (2021).
- A. Walsh and J.-S. Park, The Holey Grail of Transparent Electronics, Matter 3, 604-606 (2020).
- 21. B.-H. Jeong and <u>J.-S. Park</u>, *Calculation of stacking fault energy using anisotropic next-nearest neighbor Ising model*, New Phys.: Sae Mulli 70, 630-636 (2020).
- S. Y. Park, J.-S. Park, B. J. Kim, H. Lee, A. Walsh, K. Zhu, D. H. Kim, and H. S. Jung, Sustainable Lead Management in Halide Perovskite Solar Cells, Nature Sustainability 3, 1044–1051 (2020).

- S. Kim, S. N. Hood, J.-S. Park, L. D. Whalley, and A. Walsh, *Quick-start guide for first-principles modelling of point defects in crystalline materials*, J. Phys. Energy 2, 036001 (2020).
- 24. A. Mannodi-Kanakkithodi, J.-S. Park, A. B. F. Martinson, and M. K. Y. Chan, *Defect Energetics in Pseudo-Cubic Mixed Halide Lead Perovskites from First Principles*, J. Phys. Chem. C 124, 16729–16738 (2020).
- Ji-Sang Park, Zhenzhu Li, Jacob N. Wilson, Wan-Jian Yin, and Aron Walsh, *Hexagonal Stacking Faults Act as Hole-Blocking Layers in Lead Halide Perovskites*, ACS Energy Lett. 5, 2231–2233 (2020).
- 26. T. A. S. Doherty, A. J. Winchester, S. Macpherson, et al. Performance-limiting nanoscale trap clusters at grain junctions in halide perovskites, **Nature 580**, 360–366 (2020).
- 27. J.-S. Park, Examination of high-throughput hybrid calculations using coarser reciprocal space meshes, Curr. Appl. Phys. 20, 379-383 (2020).
- 28. K. Morita, J.-S. Park, S. Kim, K. Yasuoka, and A. Walsh, Crystal engineering of Bi₂WO₆ to polar Aurivillius-phase oxyhalides, J. Phys. Chem. C 123, **48**, 29155-29161 (2019).
- Young-Kwang Jung, Joaquín Calbo, Ji-Sang Park, Lucy Whalley, Sunghyun Kim, Aron Walsh, Intrinsic doping limit and defect-assisted luminescence in Cs₄PbBr₆, J. Mater. Chem. A 7, 20254-20261 (2019).
- 30. Ernest Pastor, **Ji-Sang Park**, Ludmilla Steier, Sunghyun Kim, Michael Grätzel, James R. Durrant, Aron Walsh, and Artem A. Bakulin, *In situ observation of picosecond polaron* self-localisation in α -Fe₂O₃ photoelectrochemical cells, Nature Commun. **10**, 3962 (2019).
- M. Sachs, J.-S. Park, E. Pastor, A. Kafizas, A. A. Wilson, L. Francàs, S.-a. Gul, M. Ling, C. Blackman, J. Yano, A. Walsh, and J. R. Durrant, *Effect of oxygen deficiency on the excited state kinetics of WO₃ and implications for photocatalysis*, Chem. Sci., 10, 5667-5677 (2019).
- Mannodi-Kanakkithodi, J.-S. Park, N. Jeon, D. H. Cao, D. J Gosztola, A. B. F. Martinson, and M. K. Y. Chan, *Comprehensive Computational Study of Partial Lead Substitution in Methylammonium Lead Bromide*, Chem. Mater. **31**, 3599-3612 (2019).
- J.-S. Park, J. Calbo, Y.-K. Jung, L. Whalley, and A. Walsh, Accumulation of Deep Traps at Grain Boundaries in Halide Perovskites, ACS Energy Lett. 4, 1321 (2019).
- F. Zhang, D. H. Kim, H. Lu, J.-S. Park, B. Larson, J. Hu, L. Gao, C. Xiao, O. Reid, X. Chen, Q. Zhao, P. F. Ndione, J. J. Berry, W. You, A. Walsh, M. C. Beard, and K. Zhu, *Enhanced Charge Transport in 2D Perovskite via Fluorination of Organic Cation*, J. Am. Chem. Soc. 141, 5972–5979 (2019).
- 35. Ji-Sang Park and Aron Walsh, Embrace your defects, Nature Energy 4, 95–96 (2019).

- Sunghyun Kim, Ji-Sang Park, Samantha N. Hood, Aron Walsh, Lone-pair effect on carrier capture in Cu₂ZnSnS₄ solar cells, J. Mater. Chem. A 7, 2686-2693 (2019).
- 37. <u>Ji-Sang Park</u>, Stabilization and self-passivation of symmetrical grain boundaries by mirror symmetry breaking, Phys. Rev. Materials **3**, 014602 (2019).
- 38. Ji-Sang Park, Youngkwang Jung, Keith Butler, and Aron Walsh, *Quick-start guide for first-principles modelling of semiconductor interfaces*, J. Phys.: Energy 1, 016001 (2019).
- Ji-Sang Park, Sunghyun Kim, Samantha H Hood, and Aron Walsh, Open-Circuit Voltage Deficit in Cu₂ZnSnS₄ Solar Cells by Interface Band Gap Narrowing, Appl. Phys. Lett. 113, 212103 (2018).
- Ji-Sang Park, Sunghyun Kim, and Aron Walsh, Stability and electronic properties of planar defects in quaternary I₂-II-IV-VI₄ semiconductors, J. Appl. Phys. **124**, 165705 (2018).
- 41. Ji-Sang Park, Sunghyun Kim, Zijuan Xie, and Aron Walsh, *Point defect engineering in thin-film solar cells*, Nature Reviews Materials **3**, 194–210 (2018).
- 42. B. Monserrat, J.-S. Park, S. Kim, and A. Walsh, *Role of electron-phonon coupling and thermal expansion on band gaps, carrier mobility, and interfacial offsets in kesterite thin-film solar cells*, Appl. Phys. Lett. **112**, 193903 (2018).
- 43. Sunghyun Kim, **Ji-Sang Park**, and Aron Walsh, *Identification of Killer Defects in Kesterite Thin-Film Solar Cells*, **ACS Energy Lett. 3**, 496–500 (2018).
- 44. Ji-Sang Park, Sunghyun Kim, and Aron Walsh, Opposing effects of stacking faults and antisite domain boundaries on the conduction band edge in kesterite quaternary semiconductors, Phys. Rev. Materials **2**, 014602 (2018).
- 45. Ji-Sang Park and Maria Chan, Mechanism of Na accumulation at extended defects in Si a first-principles study, J. Appl. Phys. **123**, 161560 (2018).
- 46. G. N. Hall, M. Stuckelberger, T. Nietzold, J. Hartman, J.-S. Park, J. Werner, B. Niesen, M. L. Cummings, V. Rose, C. Ballif, M. K. Chan, D. P. Fenning, and M. I. Bertoni, *The Role of Water in the Reversible Optoelectronic Degradation in Hybrid Perovskites at Low Pressure*, J. Phys. Chem. C, **121**, 25659–25665 (2017).
- 47. Joongoo Kang, **Ji-Sang Park**, Pauls Stradins, and Su-Huai Wei, *Nonisovalent Si-III-V and Si-II-VI alloys: Covalent, ionic, and mixed phases*, Phys. Rev. B **96**, 045203 (2017).
- D. H. Kim, J. Park, Z. Li, M. Yang, J.-S. Park, I. J. Park, J. Y. Kim, J. J. Berry, G. Rumbles, K. Zhu, 300% Enhancement of Carrier Mobility in Uniaxial-Oriented Perovskite Films Formed by Topotactic-Oriented Attachment, Adv. Mater. 29, 1606831 (2017).

- M. D. Sampson, J. S. Park, R. D. Schaller, M. K. Y. Chan, and A. B. F. Martinson, *Transition metal-substituted lead halide perovskite absorbers*, J. Mater. Chem. A 5, 3578-3588 (2017).
- 50. Zhen-Kun Yuan, Shiyou Chen, Yun Xie, Ji-Sang Park, Hongjun Xiang, Xin-Gao Gong, Su-Huai Wei, Na-Diffusion Enhanced p-type Conductivity in Cu(In,Ga)Se₂: A New Mechanism for Efficient Doping in Semiconductors, Adv. Energy. Mater. 6, 1601191 (2016).
- Ji-Hui Yang, Wan-Jian Yin, Ji-Sang Park, and Su-Huai Wei, Fast Self-Diffusion of Ions in CH₃NH₃PbI₃: the Interstiticaly Mechanism versus Vacancy-Assisted Mechanism, J. Mater. Chem. A 4, 13105-13112 (2016).)
- 52. Ji-Sang Park, Ji-Hui Yang, Teresa Barnes, and Su-Huai Wei, *Effect of intermixing at CdS/CdTe interface on defect properties*, Appl. Phys. Lett. **109**, 042105 (2016).
- 53. Ji-Hui Yang, Wan-Jian Yin, **Ji-Sang Park**, Jie Ma, and Su-Huai Wei, *Review on first-principles study of defect properties of CdTe as a solar cell absorber*, Semiconductor Science and Technology **31**, 083002 (2016).
- Ji-Sang Park, Ji-Hui Yang, Joongoo Kang, W. E. McMahon, and Su-Huai Wei, *Polymerization of defect states at dislocation cores in InAs*, J. Appl. Phys. **119**, 045706 (2016).
- Ji-Hui Yang, Wan-Jian Yin, Ji-Sang Park, Wyatt K. Metzger, and Su-Huai Wei, First-principles Study of Roles of Cu and Cl in Polycrystalline CdTe, J. Appl. Phys. 119, 045104 (2016).
- Zhen Li, Mengjin Yang, Ji-Sang-Park, Su-Huai Wei, Joseph Berry, Kai Zhu, Stabilizing Perovskite Structures by Tuning Tolerance Factor: Formation of Formamidinium and Cesium Lead Iodide Solid-State Alloys, Chem. Mater. 28, 284–292 (2016).
- Ji-Hui Yang, Wan-Jian Yin, Ji-Sang Park, and Su-Huai Wei, Self-regulation of charged defect compensation and formation energy pinning in semiconductors, Scientific Reports 5, 16977 (2015).
- 58. S. G. Choi, J.-S. Park, A. L. Donohue, B. To, C. Beall, S.-H. Wei, and I. L. Repins, *Electronic structure and optical properties of Cu₂ZnGeSe₄*: *First-principles calculations and vacuum-ultraviolet spectroscopic ellipsometric studies*, Phys. Rev. Appl. 4, 054006 (2015).
- 59. Zhen-Kun Yuan, Shiyou Chen, Hongjun Xiang, Xingao Gong, Aron Walsh, Ji-Sang Park, Ingrid Repins, Su-Huai Wei, Engineering Solar Cell Absorbers by Exploring the Band Alignment and Defect Disparity: The case of Cu and Ag-based Kesterite Compounds, Adv. Funct. Mater. 25, 6733-6743 (2015).
- 60. **Ji-Sang Park**, Sukgeun Choi, Yong Yan, Ye Yang, Joey M. Luther, Su-Huai Wei, Philip Parilla, and Kai Zhu, *Electronic Structure and Optical Properties of α*-*CH*₃*NH*₃*PbBr*₃*Perovskite Single Crystal*, **J. Phys. Chem. Lett. 6**, 4304 (2015).

- Ji-Sang Park, Bing Huang, Su-Huai Wei, Joongoo Kang, and W. E. McMahon, *Period-doubling reconstructions of semiconductor partial dislocations*, NPG Asia Materials 7, e216 (2015).
- 62. Ji-Hui Yang, Wan-Jian Yin, **Ji-Sang Park**, James Burst, Wyatt K. Metzger, Tim Gessert, Teresa Barnes, and Su-Huai Wei, *Enhanced p-type dopability of P and As in CdTe using non-equilibrium thermal processing*, J. Appl. Phys. **118**, 025102 (2015).
- I.L. Repins, J. V. Li, A. Kanevce, C. L. Perkins, K. X. Steirer, J. Pankow, G. Teeter, D. Kuciauskas, C. Beall, C. Dehart, J. Carapella, B. Bob, J.-S. Park, S.-H. Wei, *Effects of deposition termination on Cu₂ZnSnSe₄ device characteristics*, Thin Solid Films 582, 184-187 (2015).
- 64. W. H. Han, Young Jun Oh, K. J. Chang, and **Ji-Sang Park**, *Electronic structure of oxygen interstitial defects in amorphous In-Ga-Zn-O semiconductors and implications for device behavior*, Phys. Rev. Appl. **3**, 044008 (2015).
- 65. **Ji-Sang Park**, Ji-Hui Yang, Ana Kanevce, Sukgeun Choi, Ingrid L. Repins, and Su-Huai Wei, *Ordering-induced direct to indirect band gap transition in multi-cation semiconductor compounds*, Phys. Rev. B. **91**, 075204 (2015).
- 66. Ji-Hui Yang, **Ji-Sang Park**, Joongoo Kang, and Su-Huai Wei, *First-principles multi-barrier diffusion theory: The case study of interstitial diffusion in CdTe*, Phys. Rev. B **91**, 075202 (2015).
- 67. **Ji-Sang Park**, Joongoo Kang, Ji-Hui Yang, Wyatt Metzger, and Su-Huai Wei, *Stability and electronic structure of the low-* Σ grain boundaries in CdTe: a density functional study, New J. Phys. **17**, 013027 (2015).
- Ji-Sang Park, Ji-Hui Yang, Kannan Ramanathan, and Su-Huai Wei, Defect properties of Sband Bi-doped CuInSe₂: The effect of the deep lone-pair s states, Appl. Phys. Lett. **105**, 243901 (2014).
- 69. Ji-Hui Yang, **Ji-Sang Park**, Joongoo Kang, Wyatt Metzger, Teresa Barnes, and Su-Huai Wei, *Tuning the Fermi level beyond the equilibrium doping limit through quenching: The case of CdTe*, Phys. Rev. B **90**, 245202 (2014).
- 70. S. Kim, K. J. Chang, and **Ji-Sang Park**, *Finite-size supercell correction scheme for charged defects in one-dimensional systems*, Phys. Rev. B **90**, 085435 (2014).
- 71. Ji-Sang Park and K. J. Chang, Site preference of Mg acceptors and improvement of p-type doping efficiency in nitride alloys, J. Phys.: Condens. Matter. **25**, 245801 (2013).
- 72. Hyeon-Kyun Noh, **Ji-Sang Park**, and K. J. Chang, *Effect of hydrogen incorporation on the negative bias illumination stress instability in amorphous In-Ga-Zn-O thin-film-transistors*, J. Appl. Phys. **113**, 063712 (2013).

- 73. Sunghyun Kim, **Ji-Sang Park**, and K. J. Chang, *Stability and Segregation of B and P Dopants in Si/SiO*₂ *Core-Shell Nanowires*, **Nano Lett. 12**, 5068 (2012).
- 74. **Ji-Sang Park** and K. J. Chang, *Diffusion and stability of hydrogen in Mg-doped GaN: A density functional study*, Appl. Phys. Express **5**, 065601 (2012).
- 75. **Ji-Sang Park**, Byungki Ryu, and K. J. Chang, *Stability of Donor-Pair Defects in Si*_{1-x}*Ge*_x *Alloy Nanowires*, J. Phys. Chem. C **115**, 10345-10350 (2011).
- 76. Ji-Sang Park, Byungki Ryu, Chang-Youn Moon, and K. J. Chang, *Defect Responsible for the Hole Gas in Ge/Si Nanowires*, Nano Lett. **10**, 116 (2010).

PROCEEDINGS

- Arun Mannodi-Kanakkithodi, Ji-Sang Park, Duyen H. Cao, Nari Jeon, B.F. Alex Martinson, and K.Y. Maria Chan, 2018 IEEE 7th World Conference on Photovoltaic Energy Conversion (WCPEC) (A Joint Conference of 45th IEEE PVSC, 28th PVSEC & 34th EU PVSEC), DOI: 10.1109/PVSC.2018.8547974
- I. Repins, L. Mansfield, A. Kanevce, S. A. Jensen, D. Kuciauskas, S. Glynn, T. Barnes, W. Metzger, J. Burst, C.-S. Jiang, P. Dippo, S. Harvey, G. Teeter, C. Perkins, B. Egaas, A. Zakutayev, J.-H. Alsmeier, T. Lußky, L. Korte, R. G. Wilks, M. Bär, Y. Yan, S. Lany, P. Zawadzki, Ji-Sang Park, Suhuai Wei, Photovoltaic Specialists Conference (PVSC), 2016 IEEE 43rd, DOI: 10.1109/PVSC.2016.7749600
- 3. J.-S. Park, J. Kang, J.-H. Yang, W. Metzger, and S.-H. Wei, *A first-principles study of low-*Σ *grain boundaries in CdTe*, UKC 2015 conference proceedings
- 4. Ji-Sang Park, Byungki Ryu, Chang-Youn Moon, and K. J. Chang, *Hole Gas Induced by Defects in Ge/Si Core-Shell Nanowires*, AIP Conf. Proc. **1399**, 303 (2011).

INVITED PRESENTATION

- 1. Ji-Sang Park, Physical properties of grain boundaries in halide perovskites: a density functional theory calculation, 제8회 한국LED·광전자학회 학술대회, Ansan (Korea), August 8, 2022.
- 2. Ji-Sang Park, First-principles Understanding of Polycrystalline Nature of Halide Perovskites, ISPSA 2022, Jeju (Korea), July 18, 2022.
- 3. **Ji-Sang Park**, High-throughput screening of semiconductor materials for photovoltaic applications, 2022 KPS Spring Meeting, Online, April 22, 2022.
- 4. Ji-Sang Park, First-principles studies of planar defects in semiconductors for photovoltaic applications, 2021 KPS Fall Meeting, Online, October 21, 2021.
- 5. Ji-Sang Park, Computational understanding of semiconductors for photovoltaic applications, 2021 KPS Fall Meeting, Online, October 20, 2021.

- 6. **Ji-Sang Park,** High-throughput screening of semiconductor materials for photovoltaic applications, 2022 KPS Spring Meeting, Online, April 22, 2021.
- 7. **Ji-Sang Park**, First-principles studies of planar defects in semiconductors for photovoltaic applications, 2022 KPS Fall Meeting, Online, October 21, 2021.
- 8. **Ji-Sang Park**, Computational understanding of semiconductors for photovoltaic applications, 2022 KPS Fall Meeting, Online, October 20, 2021.
- 9. **Ji-Sang Park,** First-principles study of extended defects in halide perovskites, 2021 KPS Spring Meeting, Online, April 22, 2021.
- 10. **Ji-Sang Park**, First-principles studies of polytypism in semiconductors, Computational approaches to phase transitions in condensed matter, Pohang (Korea), October 7, 2020.
- 11. **Ji-Sang Park**, Segregation of defects at grain boundaries in halide perovskites, CMD2020GEFES, Strain in Metal-Halide Perovskites and other Emerging Nanomaterials (virtual conference), September 3, 2020.
- 12. **Ji-Sang Park**, Reconstruction of grain boundaries and defect accumulation, The 16th KIAS Electronic Structure Calculation Workshop (virtual Conference), August 27, 2020.
- 13. Ji-Sang Park, Stabilization and Self-passivation of Symmetrical Grain Boundary in CdTe by Mirror Symmetry Breaking, 2019년도 한국물리학회 대구경북지부 총회 및 학술발표회, Daegu (Korea), October 18, 2019.
- 14. **Ji-Sang Park**, Sunghyun Kim, and Aron Walsh, *First-principles study of extended defects in multi-component semiconductors*, Collaborative Conference on Materials Research (CCMR) 2018, Incheon (Korea), June 25-29, 2018
- 15. J.-S. Park, S. Choi, S.-H. Wei, A. Walsh, *Effect of symmetry on the electronic structure of Cu₂ZnSnSe₄ and related materials*, NEXTGEN 2017, Palma (Spain), September 12–15, 2017.
- 16. J.-S. Park, J. Kang, J.-H. Yang, W. Metzger, and S.-H. Wei, *A first-principles study of low-*Σ grain boundaries in CdTe, UKC 2015, Atlanta (USA), July 2015.
- 17. **Ji-Sang Park**, Joongoo Kang, Ji-Hui Yang, Wyatt Metzger, and Su-Huai Wei, *First-principles study of low* Σ *grain boundaries in CdTe*, APS March Meeting 2015, San Antonio (USA), March 2015.

CONTRIBUTED ORAL PRESENTATION

- 1. **Ji-Sang Park**, Prediction of the ground structure based on majority voting, 2022 KPS Spring Meeting, online (Korea), April 20, 2022.
- 2. Ji-Sang Park, First-principles studies of polytypism in semiconductors, 제12회 응용물리심포지움, online (Korea), October 15, 2021.

- 3. Kanghyeon Park, Byeong-Hyeon Jeong, **Ji-Sang Park**, *First-principles studies of stacking faults in inorganic semiconductors*, GPVC 2021, Jeju (Korea), July 8, 2021.
- 4. **Ji-Sang Park**, *Reconstruction of grain boundary in CdTe*, PVSEC-30 & GPVC 2020, Jeju (Korea), November 10, 2020.
- 5. **Ji-Sang Park**, *Hybrid density functional theory calculation for high-throughput studies*, 2020 KPS Fall Meeting, (virtual conference), November 6, 2020.
- 6. **Ji-Sang Park**, *Stabilization of grain boundaries in CdTe by mirror symmetry breaking*, 2020 KPS Spring Meeting (Korea), July 14, 2020.
- 7. **Ji-Sang Park**, *Stabilization and Self-passivation of Symmetrical Grain Boundary in CdTe by Mirror Symmetry Breaking*, 2019 E-MRS Spring Meeting, Nice (France), May 29, 2019.
- 8. **Ji-Sang Park**, *Atomistic Origins of Carrier Recombination in Grain Boundaries of Halide Perovskites*, 2019 MRS Spring Meeting, Phoenix (USA), April 24, 2019.
- 9. **Ji-Sang Park**, *Effect of Extended Defects on Electrical Properties in Earth Abundant Inorganic Materials*, 2018 MRS Fall Meeting, Boston (USA), November 28, 2018.
- Ji-Sang Park, Effect of Stacking Disorder and Metastable Polymorph on Charge Conduction in Earth-Abundant Cu₂ZnSn(S,Se)₄, 2018 MRS Fall Meeting, Boston (USA), November 28, 2018.
- 11. **Ji-Sang Park**, Atomistic insight into extended defects in Cu₂ZnSnS₄ and Cu₂ZnSnSe₄, EKC 2018, Glasgow (Scotland), August 19-24, 2018.
- 12. **Ji-Sang Park**, Sunghyun Kim, and Aron Walsh, *First-principles study of extended defects in* Cu_2ZnSnS_4 and $Cu_2ZnSnSe_4$, International Workshop on Computational Semiconductor Physics, Shanghai (China), October 20-22, 2017.
- Ji-Sang Park, Ingrid L. Repins, and Su-Huai Wei, Hybrid functional study of stability and electronic structure of Cu₂ZnSn(S,Se)₄ polytypes, ACS 249th National Meeting, Denver (USA), March 2015.
- 14. **Ji-Sang Park** and K. J. Chang, *Stability of oxygen dopants in group-III nitride alloys*, 2014 APS March meeting, Denver, CO, U.S.A., March 3-7, 2014.
- 15. **Ji-Sang Park** and K. J. Chang, *Density functional calculations for the local bonding effect on the Mg acceptor level in nitride ternary alloys*, The Korean Physical Society Spring Meeting, Daejeon (Korea), April 2013.
- 16. Ji-Sang Park and K. J. Chang, *Stability and electronic structure of Mg dopants in In-GaN alloys*, APS March Meeting, Baltimore (U.S.A.), March 2013.

- 17. **Ji-Sang Park** and K. J. Chang, *A hybrid functional study of the chemical binding and migration of hydrogen in Mg-doped GaN*, The Korean Physical Society Spring Meeting, Daejeon (Korea), April 2012.
- 18. **Ji-Sang Park** and K. J. Chang, *Hybrid functional studies of stability and diffusion of hydrogen in Mg-doped GaN*, APS March Meeting, Boston (U.S.A.), March 2012.
- Ji-Sang Park, Byungki Ryu, and K. J. Chang, *Electronic structure of donor-pair defects in* Si_{1-x}Ge_x alloy nanowires, The Korean Physical Society Spring Meeting, Daejeon (Korea), April 2011.
- 20. **Ji-Sang Park**, Byungki Ryu, and K. J. Chang, *Stability of donor-pair defects in Si*_{1-x}Ge_x alloy nanowires, APS March Meeting, Dallas (U.S.A.), March 2011.
- Ji-Sang Park, Byungki Ryu, Chang-Youn Moon, and K. J. Chang, Origin of the hole gas in Ge/Si core-shell nanowires, The Korean Physical Society Spring Meeting, Daejeon (Korea), April 2010.
- 22. Ji-Sang Park, Byungki Ryu, Chang-Youn Moon, and K. J. Chang, *Defect-driven hole gas in Ge/Si core-shell nanowires*, The 3rd BK21 Young Physicists Workshop, Seoul (Korea), January 2010.

SEMINARS

- 1. Ji-Sang Park, First-principles density functional theory calculation of materials, 한밭대학교 신소재공학과, 2021년 10월 2일
- 2. Ji-Sang Park, Computational understanding of semiconductors for photovoltaic applications: a first-principles approach, 성균관대학교 에너지과학과 (대한민국), 2021년 9월 1일.
- Ji-Sang Park, 태양전지에 쓰이는 반도체에 대한 제일원리 계산, 부산대학교 화학과 (대한민국), 2021년 5월 28일.
- 4. **Ji-Sang Park**, First-principles density functional theory calculation of halide perovskites, 강원대학교 물리학과 (대한민국), 2020년 12월 18일.
- 5. Ji-Sang Park, 태양전지에 쓰이는 반도체에 대한 제일원리 계산, 경북대학교 물리학과 (대한민국), 2019년 11월 13일.
- 6. **Ji-Sang Park**, *First-principles studies of semiconductors for solar cell applications*, Department of Physics, KAIST (Korea), April 19, 2019.
- 7. **Ji-Sang Park**, *First-principles studies of extended defects in semiconductors*, Korea Research Institute of Standards and Science (Korea), April 18, 2019.
- Ji-Sang Park, First-principles studies of semiconductors for solar cell applications, Department of Energy and Materials Engineering, Dongguk university (Korea), April 10, 2019.

- 9. Ji-Sang Park, *First-principles studies of extended defects in semiconductors*, Korea Institute for Advanced Study (Korea), April 9, 2019.
- 10. **Ji-Sang Park**, *First-principles studies of extended defects in semiconductors*, Department of Physics, Ewha Womans University (Korea), April 1, 2019.
- 11. **Ji-Sang Park**, *First-principles studies of semiconductors for solar cell applications*, Université de Lorraine (France), July 13, 2018.
- 12. **Ji-Sang Park**, *First-principles studies of semiconductors for solar cell applications*, Department of Physics, Sogang University (Korea), July 5, 2018.
- Ji-Sang Park, First-principles studies of semiconductors for solar cell applications, Department of Chemistry, Ulsan National Institute of Science & Technology (Korea), July 4, 2018.
- 14. **Ji-Sang Park**, *First-principles studies of semiconductors for solar cell applications*, Department of Emerging Materials Science, Daegu Gyeongbuk Institute of Science and Technology (Korea), July 2, 2018.
- 15. Ji-Sang Park, First-principles studies of semiconductors for solar cell applications, Department of Materials Science and Engineering, KAIST (Korea), June 27, 2018.
- 16. Ji-Sang Park, First-principles studies of semiconductors for solar cell applications, Loughborough University (UK), May 16, 2018.
- 17. Ji-Sang Park, *First-principles studies of semiconductors for solar cell applications*, School of Materials Science and Engineering, Jeonnam National University (Korea), October 25, 2017.
- 18. Ji-Sang Park, First-principles studies of semiconductors for solar cell applications, Department of Physics, University of Ulsan (Korea), October 23, 2017.
- 19. Ji-Sang Park, First-principles study of semiconductors for solar cell applications, Korea Electrotechnology Research Institute (Korea), December 1, 2016.
- 20. Ji-Sang Park, *First-principles study of semiconductors for solar cell applications*, Korea Research Institute of Standards and Science (Korea), November 29, 2016.
- 21. **Ji-Sang Park**, *First-principles study of defects in semiconductors for transistor, light emitting diode, and solar cell applications*, Korea Electrotechnology Research Institute (Korea), November 27, 2014.
- 22. Ji-Sang Park, First-principles study of defects in semiconductors for transistor, light emitting diode, and solar cell applications, Korea Research Institute of Standards and Science (Korea), November 25, 2014.

23. **Ji-Sang Park**, *First-principles study of defects in semiconductors for transistor, light emitting diode, and solar cell applications*, Graduate School of Energy, Environment, Water, and Sustainability (EEWS), KAIST (Korea), November 24, 2014.