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Research Mission

To identify and exploit structure-property relationships to design and optimize functional materials for, including but not limited to, electronic and optoelectronic applications. I explore the fundamental nature of materials including imperfections and their interaction with light. I aim to tackle technical challenges and to establish reliable theory to be able to calculate all properties of any materials via multiscale materials theory such as First-principles calculations and tight-binding modeling.

Education

- **Ph.D. in Physics:** KAIST, Republic of Korea, 2016
(*Dissertation: Theoretical study on doping efficiency in silicon nanowires* supervised by [Prof. K. J. Chang](#))
- **B.S. in Physics:** KAIST, Republic of Korea, 2010

Academic Research Experience

- **Postdoctoral Research Associate**, Department of Materials, Imperial College London, 2017 - 2020 (PI [Prof. Aron Walsh](#))
- **Postdoctoral Research Associate**, Department of Physics, KAIST, 2016 - 2017 (PI [Prof. K. J. Chang](#))
- **Undergraduate internship**, Department of Physics, University of Cambridge, 2006 (Advised by [Dr. Pietro Cicuta](#))

Technical Skill

- First-principles calculations within the Density Functional Theory (DFT) framework and tight-binding modeling
- Experience in molecular dynamics simulations and finite-difference modeling
- Experience in VASP, QE, Wannier90, LAMMPS, GULP, Phonopy, etc.
- **Programing:** Python, Julia, C/C++, FORTRAN

Extracurricular Activities

- United Nations peacekeeping mission ([UNIFIL](#))
- Swimming

Publications

1. **Sunghyun Kim**, and Aron Walsh, **Comment on “Low-frequency lattice phonons in halide perovskites explain high defect tolerance toward electron-hole recombination”**, [arXiv:2003.05394](#).
2. **Sunghyun Kim**, Samantha N. Hood, Puck van Gerwen, Lucy D. Whalley, and Aron Walsh, **CarrierCapture.jl: Anharmonic Carrier Capture**, [J. Open Source Softw. 5, 2102 \(2020\)](#).
3. **Sunghyun Kim**, José A. Márquez, Thomas Unold, and Aron Walsh, **Upper limit to the photovoltaic efficiency of imperfect crystals**, [Energy Environ. Sci. 13, 1481 \(2020\)](#).
4. Kazuki Morita, Ji-Sang Park, **Sunghyun Kim**, Kenji Yasuoka, and Aron Walsh, **Crystal Engineering of to Polar Aurivillius-Phase Oxyhalides**, [J. Phys. Chem. 123, 29155 \(2019\)](#).
5. 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 - photoelectrochemical cells**, [Nat. Comm. 10, 3962 \(2019\)](#).
6. Young-Kwang Jung, Joaquín Calbo, Ji-Sang Park, Lucy D. Whalley, **Sunghyun Kim**, and Aron Walsh, **Intrinsic doping limit and defect-assisted luminescence in** , [J. Mater. Chem. A 7, 20254 \(2019\)](#).
7. **Sunghyun Kim**, Samantha N. Hood, and Aron Walsh, **Anharmonic Lattice Relaxation during Non-radiative Carrier Capture**, [Phys. Rev. B 100, 041202\(R\) \(2019\)](#).
8. **Sunghyun Kim**, Ji-Sang Park, Samantha N. Hood, and Aron Walsh, **Lone-pair effect on carrier capture in solar cells**, [J. Mater. Chem. A 7, 2686 \(2019\)](#).
9. Ji-Sang Park, **Sunghyun Kim**, Samantha N. Hood, and Aron Walsh, **Open-circuit voltage deficit in solar cells by interface bandgap narrowing**, [Appl. Phys. Lett. 113, 212103 \(2018\)](#).
10. Ji-Sang Park, **Sunghyun Kim**, and Aron Walsh, **Stability and electronic properties of planar defects in quaternary -II-IV- semiconductors**, [J. Appl. Phys. 124, 165705 \(2018\)](#).
11. MinJoong Kim, **Sunghyun Kim**, Dong Hoon Song, Se Kwon Oh, Kee Joo Chang, and Eun Ae Cho, **Promotion of electrochemical oxygen evolution reaction by chemical coupling of cobalt to molybdenum carbide**, [Appl. Catal. B 227, 340 \(2018\)](#).
12. Ji-Sang Park, **Sunghyun Kim**, Zijuan Xie, and Aron Walsh, **Point defect engineering in thin-film solar cells**, [Nat. Rev. Mat. 3, 194 \(2018\)](#).
13. Bartomeu Monserrat, Ji-Sang Park, **Sunghyun Kim**, and Aron 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 \(2018\)](#).
14. **Sunghyun Kim**, Ji-Sang Park, and Aron Walsh, **Identification of Killer Defects in Kesterite Thin-Film Solar Cells**, [ACS Energy Lett. 3, 496 \(2018\)](#).
15. 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. Mat. 2, 014602 \(2018\)](#).
16. Woo Hyun Han, **Sunghyun Kim**, In-Ho Lee, and K. J. Chang, **Prediction of Green Phosphorus with Tunable Direct Band Gap and High Mobility**, [J. Phys. Chem. Lett. 8, 4627\(2017\)](#).
17. **Sunghyun Kim**, Woo Hyun Han, In-Ho Lee, and K. J. Chang, **Boron Triangular Kagome Lattice with Half-Metallic Ferromagnetism**, [Scientific Reports 7, 7279 \(2017\)](#).

18. Ha-Jun Sung, **Sunghyun Kim**, In-Ho Lee, and K. J. Chang, **Semimetallic carbon allotrope with topological nodal line in mixed sp-sp bonding networks**, [NPG Asia Materials 9, e361 \(2017\)](#).
19. Woo Hyun Han, Young Jun Oh, Duk-Hyun Choe, **Sunghyun Kim**, In-Ho Lee, and Kee Joo Chang, **Three-dimensional buckled honeycomb boron lattice with vacancies as an intermediate phase on the transition pathway from α -B to γ -B**, [NPG Asia Materials 9, e400 \(2017\)](#).
20. Elisabeth Pratidhina, **Sunghyun Kim**, and K. J. Chang, **Design of Dipole-Allowed Direct Band Gaps in Ge/Sn Core–Shell Nanowires**, [J. Phys. Chem. C 120, 28169 \(2016\)](#).
21. In-Ho Lee, Young Jun Oh, **Sunghyun Kim**, Jooyoung Lee, and K. J. Chang, **Ab initio materials design using conformational space annealing and its application to searching for direct band gap silicon crystals**, [Comp. Phys. Comm. 203, 110 \(2016\)](#).
22. Young Jun Oh, **Sunghyun Kim**, In-Ho Lee, Jooyoung Lee, and K. J. Chang, **Direct band gap carbon superlattices with efficient optical transition**, [Phys. Rev. B 93, 085201 \(2016\)](#).
23. Young Jun Oh, In-Ho Lee, **Sunghyun Kim**, Jooyoung Lee, and K. J. Chang, **Dipole-allowed direct band gap silicon superlattices**, [Sci. Rep. 8, 18086 \(2015\)](#).
24. In-Ho Lee, Jooyoung Lee, Young Jun Oh, **Sunghyun Kim**, and K. J. Chang, **Computational search for direct band gap silicon crystals**, [Phys. Rev. B 90, 115209 \(2014\)](#).
25. **Sunghyun Kim**, Ji-Sang Park, and K. J. Chang, **Finite-size supercell correction scheme for charged defects in one-dimensional systems**, [Phys. Rev. B 90, 085435 \(2014\)](#).
26. **Sunghyun Kim**, Ji-Sang Park, and K. J. Chang, **Stability and Segregation of B and P Dopants in Si/SiO₂ Core–Shell Nanowires**, [Nano lett. 12, 5068 \(2012\)](#).

List of References

Prof. Kee Joo Chang

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Professor Chang supervised my PhD thesis.

Prof. Aron Walsh

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Professor Walsh is my PI at Imperial College London