





Sunghyun Kim

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Research Interest

- Solar cell simulations from first-principles
- Non-radiative carrier recombination via the Shockley-Read-Hall process
- Finite-size correction for the formation energy of charged defect
- First-principles calculation and tight-binding modeling of nanostructures and defects in semiconductors
- Material design thorough computational search

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

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 - Present (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](#))

Extracurricular Activities

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

Publication

1. **Sunghyun Kim**, Ji-Sang Park, Samantha N. Hood, and Aron Walsh, “**Lone-pair effect on carrier capture in $\text{Cu}_2\text{ZnSnS}_4$ solar cells**” [arXiv:1810.11259](#)
2. Ji-Sang Park, **Sunghyun Kim**, Samantha N. Hood, and Aron Walsh, “**Open-circuit voltage deficit in $\text{Cu}_2\text{ZnSnS}_4$ solar cells by interface bandgap narrowing**” [Appl. Phys. Lett. 113, 212103 \(2018\)](#)
3. Ji-Sang Park, **Sunghyun Kim**, and Aron Walsh, “**Stability and electronic properties of planar defects in quaternary II-II-IV-VI4 semiconductors**” [J. Appl. Phys. 124 165705 \(2018\)](#)
4. 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 \(2018\)](#)
5. Ji-Sang Park, **Sunghyun Kim**, Zijuan Xie, and Aron Walsh, “**Point defect engineering in thin-film solar cells**”, [Nat. Rev. Mat. 3, 194 \(2018\)](#)
6. 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 \(2018\)](#)
7. **Sunghyun Kim**, Ji-Sang Park, and Aron Walsh, “**Identification of Killer Defects in Kesterite Thin-Film Solar Cells**”, [ACS Energy Lett. 3, 496 \(2018\)](#)
8. 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 \(2018\)](#)
9. 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\(2017\)](#)
10. **Sunghyun Kim**, Woo Hyun Han, In-Ho Lee, and K. J. Chang, “**Discovery of Half-Metallic Two-Dimensional Boron Kagome Lattice through Material Design**”, [Scientific Reports 7, 7279 \(2017\)](#)
11. Ha-Jun Sung, **Sunghyun Kim**, In-Ho Lee, and K. J. Chang, “**Semimetallic carbon allotrope with topological nodal line in mixed sp^3 - sp^2 bonding networks**” [NPG Asia Materials 9, e361 \(2017\)](#)
12. 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 \(2017\)](#)
13. 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 \(2016\)](#)
14. 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 \(2016\)](#).
15. 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 \(2016\)](#).
16. 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 \(2015\)](#).
17. 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 \(2014\)](#).
18. **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 \(2014\)](#).
19. **Sunghyun Kim**, Ji-Sang Park, K. J. Chang, “**Stability and Segregation of B and P Dopants in Si/SiO₂ Core-Shell Nanowires**”, [Nano Lett. 12, 5068 \(2012\)](#).