

Sunghyun Kim

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Research Interest

- Solar cell and battery simulations from first-principles
- Carrier lifetime and non-radiative carrier recombination via the Shockley-Read-Hall process
- First-principles calculation and tight-binding modelling of nanostructures and defects in semiconductors
- Material design thorough computational search

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](#))

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**, Samantha N. Hood, and Aron Walsh, **Anharmonic Lattice Relaxation during Non-radiative Carrier Capture** [arXiv:1904.01348](#).
2. **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** *J. Mater. Chem. A*, **7**, 2686 (2019).
3. 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).
4. Ji-Sang Park, **Sunghyun Kim**, and Aron Walsh, **Stability and electronic properties of planar defects in quaternary $\text{I}_2\text{-II-IV-VI}_4$ semiconductors** *J. Appl. Phys.* **124** 165705 (2018).
5. 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).
6. Ji-Sang Park, **Sunghyun Kim**, Zijuan Xie, and Aron Walsh, **Point defect engineering in thin-film solar cells**, *Nat. Rev. Mat.* **3**, 194 (2018).
7. 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).
8. **Sunghyun Kim**, Ji-Sang Park, and Aron Walsh, **Identification of Killer Defects in Kesterite Thin-Film Solar Cells**, *ACS Energy Lett.* **3**, 496 (2018).
9. 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).
10. 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).
11. **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).
12. Ha-Jun Sung, **Sunghyun Kim**, In-Ho Lee, and K. J. Chang, **Semimetallic carbon allotrope with topological nodal line in mixed $\text{sp}^3\text{-sp}^2$ bonding networks** *NPG Asia Materials* **9**, e361 (2017).
13. 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 $\alpha\text{-B}$ to $\gamma\text{-B}$** *NPG Asia Materials* **9**, e400 (2017).
14. 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).
15. 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).
16. 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).
17. 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).

18. 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 \(2014\)](#).
19. **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 \(2014\)](#).
20. **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 \(2012\)](#).