

# 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. Ernest Pastor, Ji-Sang Park, Ludmilla Steier, **Sunghyun Kim**, Michael Grätzel, James R. Durrant, Aron Walsh & Artem A. Bakulin, **In situ observation of picosecond polaron self-localisation in  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> photoelectrochemical cells**, *Nat. Comm.* **10**, 3962 (2019).
2. Young-Kwang Jung, Joaquín Calbo, Ji-Sang Park, Lucy D. Whalley, **Sunghyun Kim** and Aron Walsh, **Intrinsic doping limit and defect-assisted luminescence in Cs<sub>4</sub>PbBr<sub>6</sub>**, *J. Mater. Chem. A, Advance Article* (2019).
3. **Sunghyun Kim**, Samantha N. Hood, and Aron Walsh, **Anharmonic Lattice Relaxation during Non-radiative Carrier Capture**, *Phys. Rev. B* **100**, 041202(R) (2019).
4. **Sunghyun Kim**, Ji-Sang Park, Samantha N. Hood, and Aron Walsh, **Lone-pair effect on carrier capture in Cu<sub>2</sub>ZnSnS<sub>4</sub> solar cells**, *J. Mater. Chem. A* **7**, 2686 (2019).
5. Ji-Sang Park, **Sunghyun Kim**, Samantha N. Hood, and Aron Walsh, **Open-circuit voltage deficit in Cu<sub>2</sub>ZnSnS<sub>4</sub> solar cells by interface bandgap narrowing**, *Appl. Phys. Lett.* **113**, 212103 (2018).
6. Ji-Sang Park, **Sunghyun Kim**, and Aron Walsh, **Stability and electronic properties of planar defects in quaternary I<sub>2</sub>-II-IV-VI<sub>4</sub> semiconductors**, *J. Appl. Phys.* **124**, 165705 (2018).
7. 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).
8. Ji-Sang Park, **Sunghyun Kim**, Zijuan Xie, and Aron Walsh, **Point defect engineering in thin-film solar cells**, *Nat. Rev. Mat.* **3**, 194 (2018).
9. 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).
10. **Sunghyun Kim**, Ji-Sang Park, and Aron Walsh, **Identification of Killer Defects in Kesterite Thin-Film Solar Cells**, *ACS Energy Lett.* **3**, 496 (2018).
11. 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).
12. 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).
13. **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).
14. Ha-Jun Sung, **Sunghyun Kim**, In-Ho Lee, and K. J. Chang, **Semimetallic carbon allotrope with topological nodal line in mixed sp<sup>3</sup>-sp<sup>2</sup> bonding networks**, *NPG Asia Materials* **9**, e361 (2017).
15. 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  $\alpha$ -B to  $\gamma$ -B**, *NPG Asia Materials* **9**, e400 (2017).
16. 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).

17. 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 \(2016\)](#).
18. 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 \(2016\)](#).
19. 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 \(2015\)](#).
20. 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 \(2014\)](#).
21. **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 \(2014\)](#).
22. **Sunghyun Kim**, Ji-Sang Park, K. J. Chang, **Stability and Segregation of B and P Dopants in Si/SiO<sub>2</sub> Core–Shell Nanowires**, [Nano lett. 12, 5068 \(2012\)](#).