

# Sunghyun Kim

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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 - 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**, José A. Márquez, Thomas Unold, and Aron Walsh, **Upper limit to the photovoltaic efficiency of imperfect crystals**, [arXiv:1912.07889](#).
2. Kazuki Morita, Ji-Sang Park, **Sunghyun Kim**, Kenji Yasuoka, and Aron Walsh, **Crystal Engineering of  $\text{Bi}_2\text{WO}_6$  to Polar Aurivillius-Phase Oxyhalides**, *J. Phys. Chem.* **123**, 29155.
3. 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  $\alpha\text{-Fe}_2\text{O}_3$  photoelectrochemical cells**, *Nat. Comm.* **10**, 3962 (2019).
4. Young-Kwang Jung, Joaquín Calbo, Ji-Sang Park, Lucy D. Whalley, **Sunghyun Kim**, and Aron Walsh, **Intrinsic doping limit and defect-assisted luminescence in  $\text{Cs}_4\text{PbBr}_6$** , *J. Mater. Chem. A* **7**, 20254 (2019).
5. **Sunghyun Kim**, Samantha N. Hood, and Aron Walsh, **Anharmonic Lattice Relaxation during Non-radiative Carrier Capture**, *Phys. Rev. B* **100**, 041202(R) (2019).
6. **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).
7. 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).
8. 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).
9. 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).
10. Ji-Sang Park, **Sunghyun Kim**, Zijuan Xie, and Aron Walsh, **Point defect engineering in thin-film solar cells**, *Nat. Rev. Mat.* **3**, 194 (2018).
11. 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).
12. **Sunghyun Kim**, Ji-Sang Park, and Aron Walsh, **Identification of Killer Defects in Kesterite Thin-Film Solar Cells**, *ACS Energy Lett.* **3**, 496 (2018).
13. 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).
14. 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).
15. **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).
16. 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).

17. 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).
18. 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).
19. 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).
20. 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).
21. 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).
22. 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).
23. **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).
24. **Sunghyun Kim**, Ji-Sang Park, and 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).

## 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*