

Sunghyun Kim

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Research Interest

- Battery and solar cell simulations from first-principles
- Mixed ionic-electronic conduction
- Non-radiative carrier recombination via the Shockley-Read-Hall process
- 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**” *J. Mater. Chem. A*, **7**, 2686 (2019)
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).