Sunghyun Kim

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Materials Design Group
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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**, Phys. Rev. B 100, 041202(R) (2019).

2. **Sunghyun Kim**, Ji-Sang Park, Samantha N. Hood, and Aron Walsh, **Lone-pair effect on carrier capture in Cu_2ZnSnS_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 Cu_2ZnSnS_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 I_2-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 sp^3-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 α-B to γ-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/SiO_2 Core–Shell Nanowires**, Nano lett. 12, 5068 (2012).