Sunghyun Kim

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Materials Design Group
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Research Interest

- Solar cell simulations from first-principles
- Non-radiative carrier recombination via the Shockley-Read-Hall process
- Finite-size correction for the formation energy of charged defect
- 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 Cu_2ZnSnS_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 Cu_2ZnSnS_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 I2-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/SiO_2 Core–Shell Nanowires"**, Nano lett. 12, 5068 (2012).