Sunghyun Kim, PhD

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Research Interest

- Non-radiative carrier recombination via 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
- Band-unfolding for first-principles electronic structures

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)

Publication

1. Ji-Sang Park, **Sunghyun Kim**, Zijuan Xie, and Aron Walsh, **"Point defect engineering in thin-film solar cells"**, Nature Review Materials
2. **Sunghyun Kim**, Ji-Sang Park, and Aron Walsh, **"Identification of Killer Defects in Kesterite Thin-Film Solar Cells"**, ACS Energy Lett. 3 496 (2018)

3. 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)
4. 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)
5. **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)
6. 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)
7. 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)
8. 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)
9. 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).
10. 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).
11. 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).
12. 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).
13. **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).
14. **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).