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 - 2020 (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. Duk-Hyun Choe, **Sunghyun Kim**, Taehwan Moon, Sanghyun Jo, Hagyoul Bae, Seung-Geol Nam, Yun Seong Lee, and Jinseong Heo, **Unexpectedly low barrier of ferroelectric switching in HfO2 via topological domain walls**, Mater. Today (In press).

2. Lucy D. Whalley, Puck van Gerwen, Jarvist M. Frost, **Sunghyun Kim**, Samantha N. Hood, and Aron Walsh, **Giant Huang–Rhys Factor for Electron Capture by the Iodine Intersitial in Perovskite Solar Cells**, J. Am. Chem. Soc. 143, 9123–9128 (2021).

3. **Sunghyun Kim** and Aron Walsh, **Ab initio calculation of the detailed balance limit to the photovoltaic efficiency of single p-n junction kesterite solar cells**, Appl. Phys. Lett. 118, 243905 (2021).

4. Andrea Crovetto, **Sunghyun Kim**, Moritz Fischer, Nicolas Stenger, Aron Walsh, Ib Chorkendorff, and Peter C. K. Vesborg, **Assessing the defect tolerance of kesterite-inspired solar absorbers**, Energy Environ. Sci. 13, 3489-3503 (2020).

5. **Sunghyun Kim**, Samantha N. Hood, Ji-Sang Park, Lucy D. Whalley, and Aron Walsh, **Quick-start quide for first-principles modelling of point defects in crystalline materiasl**, J. Phys. Energy 2, 036001 (2020).

6. **Sunghyun Kim**, and Aron Walsh, **Comment on "Low-frequency lattice phonons in halide perovskites explain high defect tolerance toward electron-hole recombination"**, arXiv:2003.05394.

7. **Sunghyun Kim**, Samantha N. Hood, Puck van Gerwen, Lucy D. Whalley, and Aron Walsh, **CarrierCapture.jl: Anharmonic Carrier Capture**, J. Open Source Softw. 5, 2102 (2020).

8. **Sunghyun Kim**, José A. Márquez, Thomas Unold, and Aron Walsh, **Upper limit to the photovoltaic efficiency of imperfect crystals**, Energy Environ. Sci. 13, 1481 (2020).

9. Kazuki Morita, Ji-Sang Park, **Sunghyun Kim**, Kenji Yasuoka, and Aron Walsh, **Crystal Engineering of Bi_2WO_6 to Polar Aurivillius-Phase Oxyhalides**, J. Phys. Chem. 123, 29155 (2019).

10. 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 α-Fe_2O_3 photoelectrochemical cells**, Nat. Comm. 10, 3962 (2019).

11. Young-Kwang Jung, Joaquín Calbo, Ji-Sang Park, Lucy D. Whalley, **Sunghyun Kim**, and Aron Walsh, **Intrinsic doping limit and defect-assisted luminescence in Cs_4PbBr_6**, J. Mater. Chem. A 7, 20254 (2019).

12. **Sunghyun Kim**, Samantha N. Hood, and Aron Walsh, **Anharmonic Lattice Relaxation during Nonradiative Carrier Capture**, Phys. Rev. B 100, 041202(R) (2019).

13. **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).

14. 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).

15. 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).

16. 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).

17. Ji-Sang Park, **Sunghyun Kim**, Zijuan Xie, and Aron Walsh, **Point defect engineering in thin-film solar cells**, Nat. Rev. Mat. 3, 194 (2018).

18. 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).

19. **Sunghyun Kim**, Ji-Sang Park, and Aron Walsh, **Identification of Killer Defects in Kesterite Thin-Film Solar Cells**, ACS Energy Lett. 3, 496 (2018).

20. 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).

21. 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).

22. **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).

23. 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).

24. 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).

25. 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).

26. 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).

27. 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).

28. 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).

29. 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).

30. **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).

31. **Sunghyun Kim**, Ji-Sang Park, and K. J. Chang, **Stability and Segregation of B and P Dopants in Si/SiO_2 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