

# Young-Kwang Jung – *Curriculum Vitae*

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## Personal Profile

I'm a Ph.D. candidate in Materials Science and Engineering at Yonsei University. My research area is in computational materials simulation based on first-principles density functional theory (DFT). I've worked on many metal halide compounds for their uses in energy applications, e.g. Photovoltaics, LEDs, and Thermoelectrics.

## Education

**Mar 2012 -** Department of Materials Science and Engineering, Yonsei University, Seoul, Korea  
**Feb 2016** *Bachelor's Degree*

**Mar 2016 -** Department of Materials Science and Engineering, Yonsei University, Seoul, Korea  
**Aug 2021** *Doctorate Degree, Expected*  
Thesis Title – *Ab Initio* Materials Modelling: Metal Halides for Energy Applications  
Supervisor – Prof. Aron Walsh

## Research Experience

**Apr 2014 -** Materials Theory Group, Yonsei University, Seoul, Korea  
**Feb 2016** *Undergraduate Internship*

**Jul 2017 -** Department of Materials, Imperial College London, London, UK  
**Feb 2019** *Visiting Researcher (Every Summer & Winter Break)*

## Honours and Awards

**2019** Graduate School of Yonsei University – *Research Scholarship Grant*  
**2019** European Materials Research Society – *Graduate Student Award*

## Publications

(<sup>+</sup>: Equally contributed authors, \*: Corresponding authors)

1. S.-H. Yoo, J.-H. Lee, **Y.-K. Jung**, and A. Soon\*, “Exploring Stereographic Surface Energy Maps of Cubic Metals via an Effective Pair-Potential Approach”, *Phys. Rev. B* **93**, 035434 (2016)
2. **Y.-K. Jung**<sup>+</sup>, J.-H. Lee<sup>+</sup>, A. Walsh\*, and A. Soon\*, “Influence of Rb/Cs Cation-Exchange on Inorganic Sn Halide Perovskites: From Chemical Structure to Physical Properties”, *Chem. Mater.* **29**, 3181–3188 (2017)
3. G. Park<sup>+</sup>, J. Lee<sup>+</sup>, S. Moon, H. Yang, A. Giri, J. Kwak, **Y.-K. Jung**, A. Soon\*, and U. Jeong\*, “Eventual Chemical Transformation of Metals and Chalcogens into Metal Chalcogenide Nanoplates through a Surface Nucleation-Detachment-Reorganization Mechanism”, *Chem. Mater.* **29**, 3219–3227 (2017)

4. A. Kaltzoglou, C. C. Stoumpos, A. G. Kontos, G. K. Manolis, K. Papadopoulos, K. G. Papadokostaki, V. Psycharis, C. C. Tang, **Y.-K. Jung**, A. Walsh, M. G. Kanatzidis, and P. Falarasa\*, “Trimethylsulfonium Lead Triiodide: An Air-Stable Hybrid Halide Perovskite”, *Inorg. Chem.* **56**, 6302-6309 (2017)
5. L. D. Whalley, J. M. Frost, **Y.-K. Jung**, and A. Walsh\*, “Perspective: Theory and Simulation of Hybrid Halide Perovskites”, *J. Chem. Phys.* **146**, 220901 (2017)
6. **Y.-K. Jung**, K. T. Butler, and A. Walsh\*, “Halide Perovskite Heteroepitaxy: Bond Formation and Carrier Confinement at the PbS-CsPbBr<sub>3</sub> Interface”, *J. Phys. Chem. C* **121**, 27351-27356 (2017)
7. J.-S. Park, **Y.-K. Jung**, K. T. Butler, and A. Walsh\*, “Quick-Start Guide for First-Principles Modelling of Semiconductor Interfaces”, *J. Phys. Energy* **1**, 016001 (2019)
8. T. W. Jones<sup>+</sup>, A. Osherov<sup>+</sup>, M. Alsari<sup>+</sup>, M. Sponseller, B. C. Duck, **Y.-K. Jung**, C. Settens, F. Niroui, R. Brenes, C. V. Stan, Y. Li, M. Abdi-Jalebi, N. Tamura, J. E. Macdonald, M. Burghammer, V. Bulović, A. Walsh, G. J. Wilson, S. Lilliu, and S. D. Stranks\*, “Lattice Strain Causes Non-Radiative Losses in Halide Perovskites”, *Energy & Environ. Sci.* **12**, 596-606 (2019)
9. M. Shin<sup>+</sup>, J. Kim<sup>+</sup>, **Y.-K. Jung**<sup>+</sup>, T.-p. Ruoko, A. Primagi, A. Walsh\*, and B. Shin\*, “Low-Dimensional Formamidinium Lead Perovskite Architectures via Controllable Solvent Intercalation”, *J. Mater. Chem. C* **7**, 3945-3951 (2019)
10. J.-S. Park\*, J. Calbo, **Y.-K. Jung**, L. D. Whalley, and A. Walsh\*, “Accumulation of Deep Traps at Grain Boundaries in Halide Perovskites”, *ACS Energy Lett.* **4**, 1321-1327 (2019)
11. **Y.-K. Jung**, J. Calbo, J.-S. Park, L. D. Whalley, S. Kim, and A. Walsh\*, “Intrinsic doping limit and defect-assisted luminescence in Cs<sub>4</sub>PbBr<sub>6</sub>”, *J. Mater. Chem. A* **7**, 20254-20261 (2019)
12. T. A. S. Doherty<sup>+</sup>, A. J. Winchester<sup>+</sup>, S. Macpherson, D. N. Johnstone, V. Pareek, E. M. Tennyson, S. Kosar, F. U. Kosasih, M. Anaya, M. Abdi-Jalebi, Z. Andaji-Garmaroudi, E. L. Wong, J. Madéo, Y.-H. Chiang, J.-S. Park, **Y.-K. Jung**, C. E. Petoukhoff, G. Divitini, M. K. L. Man, C. Ducati, A. Walsh, P. A. Midgley, K. M. Dani\*, and S. D. Stranks\*, “Performance-limiting nanoscale trap clusters at grain junctions in halide perovskites”, *Nature* **580**, 360-366 (2020)
13. E. Welch\*, **Y.-K. Jung**, A. Walsh, L. Scolfaro, and A. Zakhidov\*, “A density functional theory study on the interface stability between CsPbBr<sub>3</sub> and CuI”, *AIP Adv.* **10**, 085023 (2020)
14. E. M. Hutter\*, L. A. Muscarella, F. Wittmann, J. Versluis, L. McGovern, H. J. Bakker, Y.-W. Woo, **Y.-K. Jung**, A. Walsh, and B. Ehrler\*, “Thermodynamic Stabilization of Mixed-Halide Perovskites against Phase Segregation”, *Cell Rep. Phys. Sci.* **1**, 100120 (2020)
15. L. A. Muscarella, E. M. Hutter, F. Wittmann, Y. W. Woo, **Y.-K. Jung**, L. McGovern, J. Versluis, A. Walsh, H. J. Bakker, and B. Ehrler\*, “Lattice Compression Increases the Activation Barrier for Phase Segregation in Mixed-Halide Perovskites”, *ACS Energy Lett.* **5**, 3152-3158 (2020)
16. **Y.-K. Jung**, I. T. Han, Y. C. Kim\*, and Aron Walsh\*, “Prediction of high thermoelectric performance in the low-dimensional metal halide Cs<sub>3</sub>Cu<sub>2</sub>I<sub>5</sub>”, *accepted in npj Comput. Mater.*
17. E. Jedlicka<sup>+</sup>, J. Wang<sup>+</sup>, J. Mutch, **Y.-K. Jung**, P. Went, J. Mohammed, M. Ziffer, R. Giridharagopal, A. Walsh, J.-H. Chu, and D. S. Ginger\*, “Bismuth-doping Alters Structural Phase Transitions in Methylammonium Lead Tribromide Single Crystals”, *under revision*
18. J.-M. Yang, **Y.-K. Jung**, J.-H. Lee, Y. C. Kim, S.-Y. Kim, D.-A. Park, J.-H. Kim, S.-Y. Jeong, J.-H. Park, I.-T. Han, A. Walsh, and N.-G. Park\*, “Memristive Cs<sub>3</sub>Cu<sub>2</sub>I<sub>5</sub> Enables Flexible, Transparent Artificial Synapse Operated at Femtojoule”, *in preparation*
19. **Y.-K. Jung**, A. Mayami, R. H. Friend, S. D. Stranks\*, and A. Walsh\*, “Pressure-Induced Carrier Recombination in Halide Perovskite Light-Emitting Diodes”, *in preparation*
20. **Y.-K. Jung**, S. Kim, and A. Walsh\*, “On the Origin of High Quantum Yield in Cs<sub>3</sub>Cu<sub>2</sub>I<sub>5</sub>: Phase Impurities, Point Defects, and Self-Trapped Excitons”, *in preparation*
21. **Y.-K. Jung** and A. Walsh\*, “PbI<sub>2</sub> Phase Impurities Trap Electrons in Lead Halide Perovskites”, *in preparation*

## Conference Presentations

- 2016** CSCT Summer Showcase *in Bath, UK* (poster) / NANOENERGY *in Liverpool, UK* (poster) / SSCG Christmas Meeting *in Loughborough, UK* (poster)
- 2017** E-MRS Spring Meeting *in Strabourg, France* (poster) / MC13 *in Liverpool, UK* (poster) / MRS Fall Meeting *in Boston, USA* (poster)
- 2018** Spring Conference of KIM *in Jeju, Korea* (oral) / CAMD Summer School *in Helsingør, Denmark* (poster) / nanoGe Fall Meeting *in Torremolinos, Spain* (oral) / MRS Fall Meeting *in Boston, USA* (oral)
- 2019** E-MRS Spring Meeting *in Nice, France* (oral) / ASIAN-22 *in Osaka, Japan* (poster) / MRS Fall Meeting *in Boston, USA* (oral)
- 2020** MRS Spring/Fall Meeting *in Virtual* (oral)

## Research Skills

### ■ Programming Languages

*Bash*  
*Python*  
*Julia*

### ■ Simulation Packages

*Electronic Structure* – VASP, Wannier90  
*Phonon* – Phonopy, Phono3py  
*Transport* – BoltzTrap2, AMSET  
*Defect* – CPLAP, SC-FERMI, CarrierCapture.jl

### ■ Miscellaneous

*Visualisation* – VESTA3  
*Graphing* – Igor Pro 8

## Hobbies and Interests

### ■ Travel

*UK* – London, Bath, Penzance, Edinburgh, Glasgow, Aberdeen, Inverness, Orkney, Shetland Islands, / *Europe* – France, Germany, Belgium, Netherlands, Italy, Portugal, Spain, Switzerland, Denmark, Monaco / *USA* – Seattle, Los Angeles, San Francisco, Boston / *Asia and Oceania* – Japan, Singapore, New Zealand

### ■ Piano

*Classic* – S. Rachmaninoff, L. v. Beethoven, F. Chopin / *New Age* – Joe Hisaishi, Yiruma

### ■ Cooking

*Italian* – Pasta, Risotto / *Korean* – Jjigae / *Western* – Steak

### ■ Drinking

*Beer* – India Pale Ale, Imperial Stout / *Wine* – Cabernet Sauvignon, Chardonnay / *Coffee* – Espresso, Latte

## Referees

**Name** Aron Walsh  
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Imperial College London  
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