

# Yoonjae Park

77 Massachusetts Avenue, Building 2, Cambridge, MA 02139, USA

Email: ypark0420@gmail.com / yoonpark@mit.edu

## RESEARCH INTERESTS

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Our research aims to develop theoretical frameworks and computational methodologies to address fundamental questions at the interface of chemistry, physics, and material science. By integrating theory, modeling, and simulation techniques—grounded in path integral theory, statistical mechanics, and quantum mechanics—we strive to uncover physical insights into complex molecular and condensed-phase phenomena.

## EDUCATION

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- **05/2023**      *Ph.D.*, Physical Chemistry, **University of California-Berkeley**, CA, USA  
 Advisor: Prof. David T. Limmer  
 Thesis: “Interplay between structural dynamics and optoelectronic properties in lead halide perovskites”
- **02/2018**      *M. S.*, Physical Chemistry, **Sogang University**, Seoul, South Korea  
 Advisor: Prof. Bong June Sung  
 Thesis: “Simulation studies on dramatically slow dynamics of glass-forming liquids and seemingly Fickian but heterogeneous dynamics of a single particle in various ways”
- **02/2016**      *B.S. Dual major in Chemistry & Mathematics, Summa Cum Laude*, Sogang University, Seoul, South Korea
- **Spring 2015**      State University of New York, Geneseo, *Exchange Student Program*

## PROFESSIONAL EXPERIENCE

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- **2023-2025**      *Postdoctoral Associate*, Chemistry, **Massachusetts Institute of Technology**, MA, USA  
 Advisor: Prof. Adam P. Willard

## PUBLICATIONS

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\* denotes equal contributions and † denotes corresponding author.

11. **Yoonjae Park** and Adam P. Willard, *Machine learning assisted entropy driven energy transport in 1-, 2-, and 3-D random lattices*, (2025) (in preparation)
10. **Yoonjae Park** and Adam P. Willard, *Extracting Electronic Coupling for Interfacial Electron Transfer via Ring Polymer Instanton Method in Condensed Phases*, (2025) (in preparation)
9. **Yoonjae Park** and Adam P. Willard<sup>†</sup>, *Modeling interfacial electron transfer using path integral molecular dynamics*, **arXiv** (2025) (submitted) <https://arxiv.org/abs/2509.17347>
8. **Yoonjae Park**, Rohit Rana, Daniel Chabeda, Eran Rabani, and David T. Limmer<sup>†</sup>, *Theoretical insights into the role of lattice fluctuations on the excited behavior of lead halide perovskites*, **Acc. Mater. Res.** (2025) (accepted)
7. **Yoonjae Park** and David T. Limmer<sup>†</sup>, *Biexcitons are bound in CsPbBr<sub>3</sub> perovskite nanocrystals*, **Phys. Rev. Materials**, 7, 106002 (2023)
6. Daniel Weinberg<sup>†</sup>, **Yoonjae Park**<sup>†</sup>, David T. Limmer<sup>†</sup>, and Eran Rabani<sup>†</sup>, *Size-dependent lattice symmetry breaking determines the exciton fine structure of perovskite nanocrystals*, **Nano Letters**, 23, 11, 4997-5003 (2023)
5. Mengyu Gao, **Yoonjae Park**, Jianbo Jin, Pengcheng Chen, Hannah Devyldere, Yao Yang, Chengyu Song, Zhenni Lin,

- Qiuchen Zhao, Martin Siron, Mary C. Scott<sup>†</sup>, David T. Limmer<sup>†</sup>, and Peidong Yang<sup>†</sup>, *Direct observation of transient structural dynamics of atomically thin halide perovskite nanowires*, **J. Am. Chem. Soc.**, 145, 4800-4807 (2023)
4. **Yoonjae Park** and David T. Limmer<sup>†</sup>, *Renormalization of excitonic properties by polar phonons*, **J. Chem. Phys.**, Editor's Choice, 157, 104116 (2022)
  3. **Yoonjae Park**, Amael Obliger, and David T. Limmer<sup>†</sup>, *Nonlocal screening dictates the radiative lifetimes of excitations in lead halide perovskites*, **Nano Letters**, 22, 2398-2404 (2022)
  2. Li Na Quan<sup>\*</sup>, **Yoonjae Park**<sup>\*</sup>, Peijun Guo, Mengyu Gao, Jianbo Jin, Jianmei Huang, Jason K. Copper, Adam Schwartzberg, Richard Schaller, David T. Limmer<sup>†</sup>, and Peidong Yang<sup>†</sup>, *Vibrational relaxation dynamics in layered perovskite quantum wells*, **Proc. Natl. Acad. Sci.**, 118 (25) e2104425118 (2021)
  1. **Yoonjae Park**, Jeongmin Kim, and Bong June Sung<sup>†</sup>, *Translation-Rotation Decoupling of Tracers of Locally Favorable Structures in Glass-Forming Liquids*, **J. Chem. Phys.** 147, 124503 (2017)

## HONORS & AWARDS

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<u>Awards</u>	<u>Years</u>
• <b>Kwanjeong Educational Foundation Fellowship</b>	08/2018 – 08/2023
• Berkeley Statistical Mechanics Meeting, <i>Excellent Poster Presentation Prize</i>	01/2022
• The Polymer Society of Korea 2016 Fall Meeting IUPAC PSK40, <i>Excellent Poster Presentation Prize</i>	10/2016
• Sogang University Graduation with Honor, <i>Summa Cum Laude</i>	02/2016
• <i>Rochester Math Olympiad 1<sup>st</sup> place</i> (the State University of New York, Geneseo)	02/2015
• Sogang University <i>Albatross Scholarship</i> (Top 10% high-grade student)	03/2016, 09/2016, 03/2017, 09/2017
• Sogang University <i>Maru Alumni Scholarship</i>	03/2015, 03/2016
• Sogang University <i>Honors Scholarship</i>	03/2014, 09/2014, 03/2015

## PRESENTATIONS

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19. Y. Park, *Interplay between structural dynamics and optoelectronic properties in lead halide perovskites*, Korea Institute of Science and Technology (KIST) (oral presentation) 06 / 2023
18. Y. Park and D. T. Limmer, *Biexcitons in lead halide perovskite nanocrystals*, APS March Meeting (oral presentation) 03 / 2023
17. Y. Park, *Path integral approach for lattice effect on excitonic properties in semiconductors*, Berkeley Kavli ENSI Research Seminar (oral presentation) 02 / 2023
16. Y. Park and D. T. Limmer, *Biexcitons in lead halide perovskite nanocrystals*, Berkeley Statistical Mechanics Meeting (poster presentation) 01 / 2023
15. Y. Park and D. T. Limmer, *Path integral approach for lattice effect on excitonic properties*, American Conference on Theoretical Chemistry 2022 (poster presentation) 07 / 2022
14. Y. Park and D. T. Limmer, *Nonperturbative lattice effects on electron-hole recombination in lead halide perovskites*, APS March Meeting (oral presentation) 03 / 2022
13. Y. Park and D. T. Limmer, *Nonlocal screening dictates the radiative lifetimes of excitations in lead halide perovskites*, Berkeley Statistical Mechanics Meeting (poster virtual presentation) 01 / 2022

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| 12. Y. Park and D. T. Limmer, <i>Electron-hole recombination in hybrid lead halide perovskites from quasiparticle path integral molecular dynamics</i> , CECAM: Path Integral Quantum Mechanics (oral virtual presentation)                    | 06 / 2021 |
| 11. Y. Park and D. T. Limmer, <i>Understanding anharmonicity in hybrid lead halide perovskites from molecular dynamics simulations</i> , APS March Meeting (oral virtual presentation)   | 03 / 2021 |
| 10. Y. Park and D. T. Limmer, <i>Vibrational dynamics in 2D layered perovskites from molecular dynamics simulations</i> , ACS Fall National Meeting (oral virtual presentation)  | 08 / 2020 |
| 9. Y. Park and D. T. Limmer, <i>Simulations on the Dynamics of Charge Carriers in Crystalline Lattice using Path Integral Framework</i> , Berkeley Statistical Mechanics Meeting (poster presentation)   | 01 / 2020 |
| 8. Y. Park and D. T. Limmer, <i>Simulations on the Dynamics of Charge Carriers in Crystalline Lattice using Path Integral Framework</i> , Telluride School on Theoretical Chemistry (poster presentation)                                      | 07 / 2019 |
| 7. Y. Park and B. J. Sung, <i>Translation-Rotation Decoupling of Tracers of Locally Favorable Structures in Glass-Forming Liquids</i> , 120 <sup>th</sup> General Meeting of the Korean Chemical Society (poster presentation)                 | 10 / 2017 |
| 6. Y. Park and B. J. Sung, <i>Translation-Rotation Decoupling of Tracers of Locally Favorable Structures in Glass-Forming Liquids</i> , The Polymer Society of Korea Fall Meeting (oral presentation)  | 10 / 2017 |
| 5. Y. Park and B. J. Sung, <i>Simulation Study on Translation-Rotation Decoupling of Tracers of Locally Favorable Structures in Glass-Forming Liquids</i> , Statistical Mechanics Symposium (oral presentation)                                | 07 / 2017 |
| 4. Y. Park and B. J. Sung, <i>Translation-Rotation Decoupling of Tracers of Locally Favorable Structures in Glass-Forming Liquids</i> , 124 <sup>th</sup> General Meeting of the Korean Physical Chemistry Society (poster presentation)       | 07 / 2017 |
| 3. Y. Park, J. Kim and B. J. Sung, <i>A Simulation Study on the Structural Motif and the Translation-Rotation Decoupling in Glass-Forming Liquids</i> , 119 <sup>th</sup> General Meeting of the Korean Chemical Society (poster presentation) | 04 / 2017 |
| 2. Y. Park, J. Kim and B. J. Sung, <i>Translational and Rotational Decoupling Using Tracers of Locally Favorable Structures in Glass-Forming Liquids</i> , Workshop on Statistical Mechanics (oral presentation)                               | 01 / 2017 |
| 1. Y. Park, J. Kim and B. J. Sung, <i>Molecular Dynamics Simulation of the Translation and Rotation Decoupling Using Tracers of Locally Favorable Structures in Binary Glass Formers</i> , IUPAC PSK40 (poster presentation)                   | 10 / 2016 |

## WORKSHOP AND PROJECT

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| • Perspective on quantum computing applications in electrochemistry, collaboration: MIT, Zapata, and Chevron | 2023-2024 |
| • 2022 School on Electron-Phonon Physics from First Principles, University of Texas, Austin                  | 06 / 2022 |
| • CECAM: Path Integral Quantum Mechanics   | 06 / 2021 |
| • Telluride School on Theoretical Chemistry  | 07 / 2019 |

## TEACHING EXPERIENCE

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|---|--------------------------|
| • Graduate Student Instructor at UC Berkeley, <i>CHM220B Advanced Statistical Mechanics</i> | Spring 2021              |
| • Graduate Student Instructor at UC Berkeley, <i>CHM120B Physical Chemistry</i>             | Spring 2020              |
| • Graduate Student Instructor at UC Berkeley, <i>CHM1A/AL General Chemistry</i>             | Spring 2019              |
| • Teaching Assistant at Sogang University, <i>CHM2201 Physical Chemistry I</i>              | Fall 2017                |
| • Teaching Assistant at Sogang University, <i>CHM1001 General Chemistry I</i>               | Spring 2016, Spring 2017 |
| • Teaching Assistant at Sogang University, <i>CHM1002 General Chemistry II</i>              | Fall 2016                |

**LEADERSHIP ACTIVITY**

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- UC Berkeley Korean Graduate Student Association 08/2019 - 08/2020
- Student Council of the Department of Chemistry, Sogang University 02/2013 - 02/2015
  - *Vice-President* (02/2014 - 02/2015)

**COMPUTER SKILL**

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- Fortran programming *Advanced*
- Python programming *Intermediate*
- Mathematica *Intermediate*
- Matlab programming *Basic*
- C language programming *Basic*