HYUNA KWON

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CURRENT PROFESSIONAL APPOINTMENT

Postdoctoral Researcher *April 2023 - Present*
Quantum Simluations Group, Lawrence Livermore National Laboratory
- Advisor: Dr. Tuan Anh Pham
- Current projects:

1) Large language model for polymer database generation;
2) Crosscutting modeling to accelerate clean energy production

EDUCATION

University of California, Riverside *September 2018 - March 2023*
PhD in Chemical and Environmental Engineering
- Advisors : Dr. De-en Jiang, Dr. Bryan M. Wong
- Thesis : Atomistic Insights into Material Chemistry: From First Principles to Machine Learning

Seoul National University *March 2014 - February 2018*
BS in Energy Resources Engineering
BS in Chemical and Biological Engineering (double majored)

Gyeonggi Science High School for Gifted *March 2011 - February 2014*

FUNDING

Research Allocation "aemdegr" | NREL HPC Systems | 240,000 AUs for FY25 | Project Lead

HONORS & AWARDS

Environmental Science & Technology Letters Best Paper Award *2023*
CCMS Internship at LLNL *June 2023 - August 2023*
Dean's distinguished fellowship *September 2018 - May 2020*
POSCO scholarship *March 2017 - February 2018*
McDonell Global Energy and Environment Partnership fellowship *June 2016 - August 2016*
Euisan superior scholarship *March 2014 - December 2014*

MENTORING & TEACHING

Teaching Assistant *September 2018 - March 2022*
- Chemistry Lab
- Transport Phenomena
- Computations for Chemical Engineering
- Advanced Thermodynamics

Mentoring Undergraduate Summer Intern
- LLNL | Data Science Initiative Summer mentoring *June 2024 - October 2024*
- University of California, Riverside | TUNE Program Summer mentoring *June 2020 - August 2020*

PUBLICATIONS

Google Scholar: Hyuna Kwon (First author: 6, Citations: 597, h-index = 12 as of 12/2024)

20 **Hyuna Kwon**, Tim Hsu, Matthew R. Carbone, Daniel Schwalbe-Koda, Fei Zhou, Deyu Lu, Tuan Anh Pham: "Multi-modal spectroscopy-guided generation of molecules via conditional diffusion model" *Under Preparation*

20 **Hyuna Kwon**, De-en Jiang: "Understanding electrooxidation of furfural on Cu, Co- spinel oxides from density functional theory" *To be submitted*

19 Bo Lei, Enze Chen, **Hyuna Kwon**, Tim Hsu, Babak Sadigh, Vincenzo Lordi, Timofey Frolov, Fei Zhou: "Grand canonical generative diffusion model for crystalline phases and grain boundaries" *Submitted*

18 **Hyuna Kwon***, Tim Hsu*, Wenyu Sun, Wonseok Jeong, Fikret Aydin, James Chapman, Xiao Chen, Matthew R. Carbone, Deyu Lu, Fei Zhou, Tuan Anh Pham: "Spectroscopy-guided generation of disordered structures via conditional diffusion model" *Machine Learning: Science & Technology*, **5**, 045037 (2024) *Equal contribution

17 **Hyuna Kwon**, Marcos Calegari, Shane Ardo, Daniel V. Esposito, Tuan Anh Pham, Tadashi Ogitsu: "Confinement Effects on Proton Transfer in TiO_2 Nanopores from Deep Potential Molecular Dynamics Simulations" *ACS Applied Materials & Interfaces*, **16**, 31687–31695 (2024)

16 **Hyuna Kwon**, Wenyu Sun, Tim Hsu, Wonseok Jeong, Fikret Aydin, Shubham Sharma, Fanchen Meng, Matthew Carbone, Xiao Chen, Deyu Lu, Liwen Wan, Michael Nielsen, Tuan Anh Pham: "Harnessing Neural Networks for Elucidating X-Ray Absorption Structure-Spectrum Relationships in Amorphous Carbon" *Journal of Physical Chemistry C*, **127**, 16473-16484 (2023)

15 **Hyuna Kwon**, Anshuman Kumar, Mauro Del Ben, Bryan M. Wong: "Electron/Hole Mobilities of Periodic DNA and Nucleobase Structures from Large-Scale DFT Calculations" *Journal of Physical Chemistry B*, **127**, 5755–5763 (2023)

14 Kaili Yan, **Hyuna Kwon**, Morgan Huddleston, De-en Jiang, Yujie Sun: "Bromonium-mediated electrochemical synthesis of 3-pyridinol from biomass-derived furfurylamine" *Journal of Physical Chemistry C*, **127**, 10107–10113 (2023)

13 **Hyuna Kwon**, De-en Jiang: "Tuning Metal-Dihydrogen Interaction in Metal-Organic Frameworks for Hydrogen Storage" *Journal of Physical Chemistry Letters*, **13**, 9129–9133 (2022)

12 **Hyuna Kwon**, Zulfikhar A. Ali, Bryan M. Wong: "Harnessing unsupervised/semi-supervised machine learning techniques to automatically predict bioactivities of per- and polyfluoroalkyl substances (PFAS)" *Environmental Science & Technology Letters*, **10**, 1017–1022 (2022)

11 Steve Yang, Zulfikhar A. Ali, **Hyuna Kwon**, Bryan M. Wong: "Predicting Complex Erosion Profiles in Steam Distribution Headers with Convolutional and Recurrent Neural Networks", *Industrial & Engineering Chemistry Research*, **61**, 8520–8529 (2022)

10 Sujan Mondal, Niket Powar, Ratul Paul, **Hyuna Kwon**, Nitumani Das, Bryan M. Wong, Su-Il In, John Mondal: "Metal-Free Porous Polyketone as Photocatalytic Assemblies for Artificial Photosynthesis", *ACS Applied Materials & Interfaces*, **14**, 771–783 (2021)

9 Prithwish Biswas, Pankaj Ghildiyal, **Hyuna Kwon**, Haiyang Wang, Zaira Alibay, Feiyu Xu, Yujie Wang, Bryan M. Wong, Michael Zachariah: "Rerouting pathways of solid-state ammonia borane energy release", *Journal of Physical Chemistry C*, **126**, 48–57 (2021)

8 Sharma S.R.K.C. Yamijala, **Hyuna Kwon**, Juchen Guo, Bryan M. Wong: "Stability of Calcium Ion Battery Electrolytes: Predictions from Large-Scale Ab Initio Molecular Dynamics Simulations", *ACS Applied Materials & Interfaces*, **13**, 13114-13122 (2021)

7 Sohag Biswas, **Hyuna Kwon**, Kelley Barsanti, Nanna Myllys, James N. Smith, Bryan M. Wong: "Ab Initio Metadynamics Calculations of Dimethylamine for Probing pK_b Variations in Bulk vs. Surface Environments", *Physical Chemistry Chemical Physics*, **22**, 26265-26277 (2020)

6 Michael Bentel, Yaochun Yu, Lihua Xu, **Hyuna Kwon**, Zhong Li, Bryan Wong, Yujie Men, Jinyong Liu: "Degradation of Perfluoroalkyl Ether Carboxylic Acids (PFECAs) with Hydrated Electrons: Structure-Reactivity Relationships and Environmental Implications", *Environmental Science & Technology*, **54**, 2489-2499 (2020)

5 Akber Raza, Sharmistha Bardhan, Lihua Xu, Chao Lian, **Hyuna Kwon**, Jinyong Liu, Bryan M. Wong: "A Machine Learning Approach for Predicting Defluorination of Per- and Polyfluoroalkyl Substances (PFAS) for Their Efficient Treatment and Removal", *Environmental Science & Technology Letters*, **6**, 624-629 (2019)

4 Chao Lian, Zulfikhar A. Ali, **Hyuna Kwon**, Bryan M. Wong : "Indirect but Efficient: Laser-Excited Electrons Can Drive Ultrafast Polarization Switching in Ferroelectric Materials", *The Journal of Physical Chemistry Letters*, **10**, 3402-3407 (2019)

3 Qisheng Jiang, Deoukchen Ghim, Sisi Cao, Sirimuvva Tadepalli, Keng-Ku Liu, **Hyuna Kwon**, Jingyi Luan, Yujia Min, Young-Shin Jun, and Srikanth Singamaneni. "Photothermally active reduced graphene oxide/bacterial nanocellulose composites as biofouling-resistant ultrafiltration membranes." *Environmental Science & Technology*, **53**, 412-421 (2018)

2 Taisei Kobayashi, Kosuke Kuroda, SeongWoo Jeong, **Hyuna Kwon**, Chunyu Zhu, Hiroki Habazaki, and Yoshitaka Aoki. "Analysis of the Anode Reaction of Solid Oxide Electrolyzer Cells with $BaZr_{0.4}Ce_{0.4}Y_{0.2}O_{3-\delta}$ Electrolytes and $Sm_{0.5}Sr_{0.5}CoO_{3-\delta}$ Anodes." *Journal of The Electrochemical Society*, **165**, F342 (2018)

1 Seongwoo Jeong, Taisei Kobayashi, Kosuke Kuroda, **Hyuna Kwon**, Chunyu Zhu, Hiroki Habazaki, and Yoshitaka Aoki. "Evaluation of thin film fuel cells with Zr-rich $BaZr_xCe_{0.8-x}Y_{0.2}O_3$ electrolytes ($x \geq 0.4$) fabricated by a single-step reactive sintering method." *RSC Advances*, **8**, 26309-26317 (2018)

INVITED SEMINARS

Ewha Women's University, "Machine Learning in Materials Discovery: Unraveling 3D Structures and Spectroscopy Insights." Host: Dr. Jonggeol Na, (May 2024)

KENTECH (Korea Institute of Energy Technology), "Machine Learning in Materials Discovery: Unraveling 3D Structures and Spectroscopy Insights." Host: Dr. Geunho Gu, (May 2024)

Brookhaven National Laboratory, "Spectroscopy-guided generation of disordered structures via conditional diffusion model." Host: Dr. Deyu Lu, (Jan 2024)

ORAL PRESENTATIONS

ECS PRiME 2024, "Proton Transfer in Nanoporous TiO_2 Films: Insights from Deep Potential Molecular Dynamics Simulations." Honolulu, HI (oral).

MRS Fall 2023, "Proton Transfer in Nanoporous TiO_2 Films: Insights from Deep Potential Molecular Dynamics Simulations." Boston, MA (oral).

MRS Fall 2023, "Spectroscopy-guided generation of disordered structures via conditional diffusion model." Boston, MA (oral).

MRS Spring 2023, "Harnessing Neural Networks for Elucidating X-Ray Absorption Structure-Spectrum Relationships in Amorphous Carbon." San Francisco, CA (oral).

ACS Spring 2022, "Understanding electrooxidation of furfural on Cu, Co- spinel oxides from density functional theory." San Diego, CA (oral).

EMPLOYMENT

ASML December 2017 - June 2018
Customer Service Engineer

POSCO December 2016 - January 2017
Intern

REFERENCES

Dr. Tuan Anh Pham, Staff Scientist, Lawrence Livermore National Laboratory, pham16@llnl.gov

Prof. De-en Jiang, Professor, Vanderbilt University, de-en.jiang@vanderbilt.edu

Prof. Deyu Lu, Staff Scientist, Brookhaven National Laboratory, dlu@bnl.gov

Daniel V. Esposito, Professor, Columbia University, de2300@columbia.edu

Prof. Young-shin Jun, Professor, Washington University in St. Louis, ysjun@wustl.edu