HYUNA KWON, PH.D.

Dublin, CA 94568

(951) 386 5344 ⋄ hyukwo@gmail.com ⋄ kwon11@llnl.gov

EDUCATION

University of California, Riverside   *September 2018 - March 2023*
PhD candidate in Chemical and Environmental Engineering
- Advisors : **Dr. De-en Jiang**, Dr. Bryan M. Wong
- Research area : **Density functional theory, Ab-initio molecular dynamics, Deep learning in materials discovery, Cheminformatics, Computational materials science**

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*

WORK EXPERIENCES

Lawrence Livermore National Lab   April 2023 - present
Postdoctoral Researcher

- Mentor : Tuan Anh Pham
- Postdoctoral researcher at Quantum Simulation Group
- Applied deep learning to predict chemical structures based on XANES (X-ray absorption near edge structure) spectra

Lawrence Livermore National Lab   June 2022 - March 2023
Intern

- Mentor : Tuan Anh Pham
- Research intern at Quantum Simulation Group of Computational Chemistry & Materials Science (CCMS) Summer Institute.
- Applied deep learning to predict chemical structures based on XANES (X-ray absorption near edge structure) spectra

University of California, Riverside   September 2018 - March 2023
Graduate student researcher

- Advisors : De-en Jiang, Bryan M. Wong
- Published 10 papers in computational chemistry field (2 first-authored)
- Applied DFT (density functional theory) and AIMD (ab-initio molecular dyanmics) to elucidate reaction mechanisms of energy storage systems.
- Experienced in modeling various systems including biological (DNA), environmental (PFAS, water aerosol), and chemical (Ca-ion batteries, spinel oxide catalysis) systems.

ASML   December 2017 - June 2018
Customer Service Engineer

- Received training required for lithography engineers.
- Was responsible for the maintenance of lithography equipment in Samsung fab.

POSCO   December 2016 - January 2017
Intern

- Proposed a new project to remove water from mixed gas in the steel making process using thermoelectric materials.
- Was awarded a POSCO scholarship for two years and got an offer for a permanent position.

Seoul National University   September 2017 - December 2017
Research Assistant

- Advisor : Taeghwan Hyeon
- Water based synthesis of FeOH nanoparticles

Hokkaido University   January 2017 - February 2017
Research Assistant

- Advisors : Yoshitaka Aoki, Hiroki Habazaki
- Papers 1 and 2 in Publications list
- Fabricated and performed the characterization of BZCY622 fuel cells

Washington University in St.Louis   June 2016 - August 2016
Research Assistant

- Advisor : Youngshin Jun
- Paper 3 in Publications list
- Fabrication of graphene oxide/biological nanocellulose membranes for water purification to prevent bio-fouling

PUBLICATIONS

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

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*, **In Press**

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* **In Press**

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**, 24, 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**, 1, 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**, 1, 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)

———————————————————————————————————————

HONORS & AWARDS

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 (Chem Lab 01LA)	*January 2022 - March 2022*
Tune Summer mentoring (Olawale Olatunde, Muslim Rana)	*June 2020 - August 2020*
Riverside high school mentor (Usha Maya Kademani)	*January 2021 - August 2021*
Undergraduate student mentoring (Anagha Belavadi)	*January 2021 - March 2021*