

# Choah Kwon

Ph.D

Email: kwonchoah@gmail.com

## EDUCATION

---

Ph.D. in Department of Chemical & Biomolecular Engineering, Yonsei University (2016. 09. - 2021. 02., Advisor: Prof. Byungchan Han)

Research Internship (2016.03 – 2016.08)

B.S. in Department of Chemical & Biomolecular Engineering, Yonsei University (2011.03 – 2016.02)

## RESEARCH INTEREST

---

1. Material informatics: combining machine learning method and first-principles calculations
2. Computational radiochemistry: electro-physicochemical properties of lanthanide and actinide elements under various environments to apply disposal of spent nuclear fuel
3. Sustainable energy resources: electro-physicochemical properties of nuclear fuel, battery and fuel cell

## RESEARCH TOPIC

---

Machine learning & AI based computational radiochemistry

## PUBLICATIONS

---

-Total publication : 9 paper

-Publication as First Author: 7 paper

1. Choah Kwon, Yi Xia, Fei Zhou and Byungchan Han, Dominant Effects of Anharmonic on the Equation of State and Thermal Conductivity for MgO under Extreme Conditions, Physical Review B, 102, 184309 (2020)
2. Changjoon Keum, Hyesung Lee, Choah Kwon, Byungchan Han and Sang-Yup Lee, A Metal-induced Self-assembly Template for Controlled Growth of ZIF-8 Nanorods, Chemistry of Materials, 32, 18, 7941-7950 (2020)
3. Choah Kwon, Kwanpyung Lee, Byungchan Han, First-Principles Study on Thermodynamic Stability of UO<sub>2</sub> with He Gas Incorporation via Alpha-Decay, Korean Chemical Engineering Research, 57(3), 1-4 (2019)

4. Jeongmook Lee, Choah Kwon, Jandee Kimm Young-Sang Youn, Joung-Yun Kim, Byungchan Han, Integrated study of experiment and first-principles computation for the characterization of a corium type  $ZrO_8$  complex in a Zr-doped fluorite  $UO_2$ , International Journal of Energy Research, 43(8) 3322-3329 (2019) \* J. Lee and C. Kwon have contributed equally to this work, **(Top journal of nuclear science & technology field)**
5. Choah Kwon, Joonhee Kang, Seung Hyo Noh, Byungchan Han, First-principles prediction of universal relation between exchange current density and adsorption energy of rare-earth elements in a molten salt, Journal of Industrial and Engineering Chemistry, 70, 94-98 (2019)
6. Choah Kwon, Seung Hyo Noh, Hoje Chun, Il Soon Hwang, Byungchan Han, First principles computational studies of spontaneous reduction reaction of Eu(III) in eutectic LiCl-KCl molten salt, International Journal of Energy Research, 42(8), 2757-2765 (2018), **(Top journal of nuclear science & technology field)**
7. Seung Hyo Noh, Jeemin Hwang, Choah Kwon, Byungchan Han, Self-assembled nitrogen-doped fullerenes and their catalysis for fuel cell and rechargeable metal–air battery applications, Nanoscale, 9(22), 7373-7379 (2017)
8. Choah Kwon, Joonhee Kang, Byunchan Han, First-principles based computational study on nucleation and growth mechanisms of U on Mo(110) surface solvated in an eutectic LiCl–KCl molten salt, International Journal of Energy Research, 40(10), 1381-1388 (2016), **(Top journal of nuclear science & technology field)**
9. Choah Kwon, Joonhee Kang, Woojong Kang, Dohyun Kwak, Byungchan Han, First principles study of the thermodynamic and kinetic properties of U in an electrorefining system using molybdenum cathode and LiCl-KCl eutectic molten salt, Electrochimica Acta, 195, 216-222 (2016)

#### AWARDS

---

1. Best poster award at NANO KOREA, 2018
2. Best poster award at Korean Electrochemical Society, 2018
3. Best presentation award at Korean Radioactive Waste Society, 2018
4. Best presentation award at Korean Institute of Hazardous Materials, 2019