NANO KOREA 2020
July 1~3, KINTEX, Korea

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EDUCATION

University of California, Berkeley	Ph.D	in Chemistry	**2005**
Iowa State University	MS	in Chemistry	**2001**
Seoul National University	MS	in Chemistry	**1999**
Seoul National University	BS	in Oceanography	**1997**

PROFESSIONAL ACTIVITIES

- Professor, Department of Chemical and Biomolecular Engineering, KAIST, Korea (March 2020 to present)
- Professor, Graduate School of EEWS, KAIST, Korea (March 2018 to Feb 2020)
- Associate Professor, Graduate School of EEWS, KAIST, Korea (September 2012 to February 2018)
- Assistant Professor, Graduate School of EEWS, KAIST, Korea (March 2009 to August 2012)
- Visiting Associate, California Institute of Technology, USA (July 2010 to July 2011)
- Postdoc, California Institute of Technology, USA (November 2005 to February 2009)

AWARD AND HONORS

- Pople Medal, Asia-Pacific Association of Theoretical and Computational Chemists (APATCC), 2018
- Young Physical Chemist Awards (Korean Chemical Society), 2017
- CSJ Distinguished Lectureship Award (Chemical Society of Japan), 2015
- Samsung Humantech Gold Prize (with Heejin Kim) (Samsung Electronics), 2014
- KCS-Wiley Young Chemist Award (Korean Chemical Society & Wiley), 2013
- US-Korea Nanoforum Gold Poster Award (NSF), 2011
- James W. Glanville Postdoctoral Fellowship (Caltech), 2007~2009
- Samsung Humantech Bronze Prize (Samsung Electronics), 2006
- IBM Graduate Student Award in Computational Chemistry (American Chemical Societcy), 2005

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MAIN SCIENTIFIC PUBLICATION

1) Inverse Design of Solid State Materials via a Continuous Representation, ***Matter*** 1, 1370 (2019)
2) Nitrogen Fixation by Ru Single-Atom Electrocatalytic Reduction, ***Chem*** 5, 204 (2019)
3) Boosting hot electron flux and catalytic activity at metal–oxide interfaces of PtCo bimetallic nanoparticles, ***Nature Comm*** 9, 2235 (2018)
4) Adsorbate-driven reactive interfacial Pt-NiO1-x nanostructure formation on the Pt3Ni(111) alloy surface, ***Science Adv*** 4, eaat3135 (2018)
5) Nanostructuring one-dimensional and amorphous lithium peroxide for high round-trip efficiency in lithium-oxygen batteries, ***Nature Comm*** 9, 680 (2018)
6) Single-atom catalysts for CO2 electroreduction with significant activity and selectivity improvements, ***Chem Sci*** 8, 1090 (2017)
7) Defect-Controlled Formation of Triclinic Na2CoP2O7 for 4V Sodium-Ion Batteries, ***Angew Chem Int Ed*** 55, 1 (2016)
8) Carbon nanofluidics of rapid water transport for energy applications, ***Chem Soc Rev*** 43, 565 (2014)
9) Role of Intermediate Phase for Stable Cycling of $Na_7V_4(P_2O_7)_4PO_4$ in Sodium Ion Battery, ***Proc Natl Acad Sci*** 111, 599 (2014)
10) Hydrogen-Bond-Assisted Controlled C-H Functionalization via Adaptive Recognition of a Purine Directing Group, ***J Am Chem Soc*** 136, 1132 (2014)
11) Strengthening effect of a single atomic layer graphene in metal-graphene nanolayered composite, ***Nature Commun*** 4, 2114 (2013)
12) Anomalous Manganese Activation of a Pyrophosphate Cathode in Sodium Ion Batteries: A Combined Experimental and Theoretical Study, ***J Am Chem Soc*** 135, 2787-2792 (2013)
13) Rollover Cyclometalation Pathway in Rhodium Catalysis: Dramatic NHC Effects in the C-H Bond Functionalization, ***J Am Chem Soc*** 138, 17778-17788 (2012)
14) Site-Specific Transition Metal Occupation in Multicomponent Pyrophosphate for Improved Electrochemical and Thermal Properties in Lithium Battery Cathodes: A Combined Experimental and Theoretical Study, ***J Am Chem Soc*** 134, 11740-11748 (2012)
15) A fast doubly hybrid density functional method close to chemical accuracy using a local opposite spin ansatz, ***Proc Natl Acad Sci*** 108, 19896-19900 (2011)
16) Entropy and the driving force for the filling of carbon nanotubes with water, ***Proc Natl Acad Sci*** 108, 11794 (2011)
17) Comment on "Inaccuracy of density functional theory calculations for dihydrogen binding energetics onto Ca cation centers", ***Phys Rev Lett*** 104, 179601 (2010)

RESEARCH INTERESTS

- Machine learning for materials design
- Developments of density functional methods and their applications for materials design
- Catalysis, Energy Storage and Conversion