Jun Huo

Master

School of Petroleum and Chemical Engineering, Dalian University of Technology No.2 Linggong Road, Ganjingzi District, Dalian City, Liaoning Province, P.R.China

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Education

Sep. 2016 - Present M.S. in Chemical Engineering

School of Petroleum and Chemical Engineering,

Dalian University of Technology

Sep. 2012 - Jul. 2016 **B.Eng.** in Chemical Engineering and Technology

College of Chemistry, Chemical Engineering and Environmental

Engineering, Liaoning Shihua University

Research Interests

Combining Machine Learning and Molecular Simulation to study polymer structure

Publications

- * indicates co-first author.
 - Jun Huo, Wenxu Qi, Hongda Zhu, et al., Molecular Dynamics Simulation on the Effect of Water Uptake on Hydrogen Bond Network for OH⁻ Conduction in Imidazolium-g-PPO Membrane, *International Journal of Hydrogen Energy*, 2019, 44: 3760–3770. doi:10.1016/j.ijhydene.2018.12.090
 - Ning Zhang, Boyun Yang, Jun Huo, et al., Hydration Structures of Vanadium/Oxovanadium Cations in the Presence of Sulfuric Acid: A Molecular Dynamics Simulation Study, Chemical Engineering Science, 2019, 195: 683-692. doi:10.1016/j.ces.2018.10.014
 - 4. Ning Zhang*, **Jun Huo***, Boyun Yang, et al., Understanding of Imidazolium Group Hydration and Polymer Structure for Hydroxide Anion Conduction in Hydrated Imidazolium-g-PPO Membrane by Molecular Dynamics Simulations, *Chemical Engineering Science*, **2018**, 192: 1167–1176.

doi:10.1016/j.ces.2018.08.051

3. Yuechun Song, **Jun Huo**, Ning Zhang, et al., Structural Characteristics of Hydrated Protons in Ion Conductive Channels: Synergistic Effect of the Sulfonate Group and Fluorine Studied by Molecular Dynamics Simulation, *The Journal of Physical Chemistry C*, **2018**, 122(4): 1982-1989.

doi:10.1021/acs.jpcc.7b11020

 Ning Zhang, Shaomin Chen, Boyun Yang, Jun Huo, et al., Effect of Hydrogen-Bonding Interaction on the Arrangement and Dynamics of Water Confined in a Polyamide Membrane: A Molecular Dynamics Simulation, *The Journal of Physical Chemistry B*, 2018, 122(17): 4719-4728.

doi:10.1021/acs.jpcb.7b12790

 Ning Zhang, Yuechun Song, Jun Huo, et al., Formation Mechanism of the Spiral-Like Structure of a Hydrogen Bond Network Confined in a Fluorinated Nanochannel: A Molecular Dynamics Simulation, *The Journal of Physical Chemistry C*, 2017, 121(25): 13840-13847.

doi:10.1021/acs.jpcc.7b01074

Papers submitted/under revision

1. **Jun Huo**, Wenxu Qi, Gaohong He, et al., Structural Characteristics of Hydrated Protons in the Conductive Channels: Effect of Electric Field Studied by Molecular Dynamics Simulation, *Nanoscale*. (Under revison)

Skills

Languages Mandarin Chinese, English.

Programming Python, C/C++, Tcl/Tk, Fortran, LaTeX, etc.

Software NAMD, Lammps, VMD, Materials Studio, Gaussian, Office, Photoshop, etc.

Awards

2018 - 2019	The First Prize of Excellent Master Degree Scholarship
2017 - 2018	The First Prize of Excellent Master Degree Scholarship
2016 - 2017	Outstanding Graduate Student Leader
2014 - 2015	Liaoning Provincial Government Scholarship
2013 - 2014	Outstanding Student Leader

Experience

Sep. 2016 - Present	Natural Science Foundation of China Research on the structure and formation mechanism of hydrated proton in the ion transport channel of proton exchange membrane.
Sep. 2016 - July. 2017	Director of Publicity Department, the Graduate Student Union
Sep. 2016 - July. 2017	College Office Assistant
Sep. 2014 - July. 2015	Director of Publicity Department, the Student Union