

# Jun Huo

## Master

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## Education

- Sep. 2016 - Present     **M.S.** in Chemical Engineering  
School of Petroleum and Chemical Engineering,  
**Dalian University of Technology**  
GPA : 3.68 / 4.0
- Sep. 2012 - Jul. 2016     **B.Eng.** in Chemical Engineering and Technology  
College of Chemistry, Chemical Engineering and Environmental  
Engineering, **Liaoning Shihua University**  
GPA : 3.50 / 4.0, Rank : 2 / 318

## Research Interests

- Combing Machine Learning Algorithm and Molecular Simulation

## Publications

\* indicates co-first author.

6. **Jun Huo**, Wenxu Qi, Hongda Zhu, et al., Molecular Dynamics Simulation on the Effect of Water Uptake on Hydrogen Bond Network for OH<sup>-</sup> Conduction in Imidazolium-g-PPO Membrane, *International Journal of Hydrogen Energy*, **2019**, 44: 3760–3770. DOI:[10.1016/j.ijhydene.2018.12.090](https://doi.org/10.1016/j.ijhydene.2018.12.090)
5. 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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1021/acs.jpcc.7b11020)
2. 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](https://doi.org/10.1021/acs.jpcb.7b12790)

1. 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](https://doi.org/10.1021/acs.jpcc.7b01074)

## Papers submitted / under review

\* indicates co-first author.

2. Daishuang Zhang\*, **Jun Huo**\*, Ning Zhang, et al., Continuous Two-Dimensional Channels Devised with Ångström-Scale Precision for Flow Batteries, *Journal of Materials Chemistry A*. (Submitted)
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 revision)

## Papers in Preparation

1. **Jun Huo**, En Jiang, Lili Huang, et al., Removal of Heavy Metals from Water across Multilayer Amino-functionalized Graphene Membranes: A Molecular Dynamics Simulation.

## Skills

<b>Languages</b>	Python, C/C++, Tcl/Tk, etc.
<b>Softwares</b>	VMD, NAMD, LAMMPS, Materials Studio, Gaussian, Office, L <sup>A</sup> T <sub>E</sub> X, Photoshop, Maya, etc.

## Awards

2019	Honorable Mention of Mathematical Contest In Modeling
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

Dec. 2018 - Present	<b>Natural Science Foundation of China</b> Multi-region dynamic ion coarse grained model based on hydrated ion structure.
Sep. 2016 - Present	<b>Natural Science Foundation of China</b> Research on the structure and formation mechanism of hydrated proton in the ion transport channel of proton exchange membrane.
Sep. 2016 - July. 2017	<b>Director of Publicity Department, the Graduate Student Union</b>
Sep. 2016 - July. 2017	<b>College Office Assistant</b>
Sep. 2014 - July. 2015	<b>Director of Publicity Department, the Student Union</b>