

# 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**
- 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.

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.jpcc.7b12790](https://doi.org/10.1021/acs.jpcc.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 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 revision)

## Skills

|                    |  |
|--------------------|--|
| <b>Languages</b>   | Mandarin Chinese, English.   |
| <b>Programming</b> | Python, C/C++, Tcl/Tk, Fortran, L <sup>A</sup> T <sub>E</sub> X, etc.  |
| <b>Software</b>    | NAMD, LAMMPS, VMD, Materials Studio, Gaussian, Office, Photoshop, etc. |

## Awards

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|-------------|--|
| 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

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|------------------------|--|
| Sep. 2016 - Present    | <b>Natural Science Foundation of China</b><br>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>   |