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** GPA : 3.48 / 4.0 (GPA-weighting algorithm) , Rank : 2 / 318

Research Interests

- Combing Machine Learning Algorithm and Molecular Simulation
- Coarse-Grained Molecular Dynamics
- *Ab initio* Molecular Dynamics

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^- Conduction in Imidazolium-g-PPO Membrane, *International Journal of Hydrogen Energy*, **2019**, 44: 3760–3770. DOI: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

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

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

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

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 revison)

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

Languages	Python, C/C++, Tcl/Tk, etc.
Softwares	NAMD, Lammps, VMD, Materials Studio, Gaussian, Office, LaTeX, Photoshop, Maya, 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

Dec. 2018 - Present	**Natural Science Foundation of China** Multi-region dynamic ion coarse grained model based on hydrated ion structure.
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**