

Jian Huang

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Education

- 2021–present **PhD, Computational Chemistry**, *UMass Amherst*, MA, Advisor: Jianhan Chen.
Computational Biophysics, Activation mechanisms of ion channels, ion channel-lipid interactions
- 2016–2019 : **Master of Biochemistry and Molecular Biology**, *University of Chinese Academy of Sciences*, Beijing, China.
Artificial photoenzyme, Genetic codon expansion, Charge separation in fluorescent protein
- 2012–2016 : **Bachelor of Applied Chemistry**, *Huazhong University of Science & Technology*, Wuhan, China.

Research

Lipid-ion channel interactions

Lipids, especially PIP2, have been shown to play important regulatory effects on many ion channels, such as TRPV4. TRPV4 is a temperature-sensitive ion channel, and it cannot be activated if PIP2 is depleted from the membrane. The mechanism behind PIP2 regulation of TRPV4 and also the binding site of PIP2 on TRPV4 is still unknown. By using docking, I found a plausible binding pocket. Now, I am trying to use MD simulations to resolve PIP2-induced conformational and dynamics changes.

Hydrophobic gating in bundle-crossing ion channels

Many ion channels can use a bundle-crossing gate to block ion current. Recently, hydrophobic dewetting provides a new mechanism for channels to block currents. The hydrophobicity in a confined pore favors lipid to vapor transition and results in a vapor bubble, which can function as a blockage. In my study of TRPV4, a temperature-sensitive channel, the pore has both features: a bundle-crossing gate and highly hydrophobic pore. Using MD simulations, I found the pore can easily form a vapor phase and disrupting the pore environment with a hydrophilic mutation can decrease the free energy barrier by a half.

Activation mechanisms of ion channels

TMEM16F is a dual-functional ion channel which involves in breaking down lipid asymmetry signaling downstream events by scrambling lipids across the bilayer. The open structure of this channel remains unrevealed, preventing us from understanding the activation process. I exploited mutations that result in constitutively open channels and used MD simulations to predict the open state and more importantly the activation mechanism.

Publications

- 2023 **Jian Huang** and Jianhan Chen. Hydrophobic gating in bundle-crossing ion channels: a case study of trpv4. *in preparation*, 2023.
- 2022 **Jian Huang**#, Zhiguang Jia#, and Jianhan Chen. Activation of tmem16f by inner gate charged mutations and possible lipid/ion permeation mechanisms. *Biophysical Journal*, 2022.
- 2021 Ting Xue, Weikun Wu, Ning Guo, Chengyong Wu, **Jian Huang**, Lipeng Lai, Hong Liu, Yalun Li, Tianyuan Wang, and Yuxi Wang. Single point mutations can potentially enhance infectivity of SARS-CoV-2 revealed by in silico affinity maturation and spr assay. *RSC Adv*, 2021.

- 2021 **Jian Huang**[#], Yu Fu[#], Yuzhou Wu, Xiaohong Liu, Fangrui Zhong, and Jiangyun Wang. Biocatalytic cross-coupling of aryl halides with a genetically engineered photosensitizer artificial dehalogenase. *J Am Chem Soc*, 2021.

Fellowships & Awards

- 2022 **Chemistry-Biology Interface Traineeship**, University of Massachusetts Amherst and National Institutes of Health
- 2015 **National Scholarship**, Ministry of Education of the People's Republic of China
- 2014 – 2015 **Merit Student**, Huazhong University of Science & Technology
- 2013 **Scholarship of Academic Excellence**, Huazhong University of Science & Technology

Talks & Posters

- 2023 **Poster** in *Biophysical Society Annual Meeting*, "Hydrophobic gating in bundle-crossing ion channels: a case study of TRPV4"
- 2022 **Talk** in *University of Massachusetts Amherst, Chemistry-Biology Interface*, "Hydrophobic gating in ion channels"
- 2022 **Poster** in *University of Massachusetts Amherst, ResearchFest*, "How does TRPV4 regulate ion permeation"
- 2022 **Poster** in *Biophysical Society Annual Meeting*, "Activation of TMEM16F by inner gate charged mutations & mechanisms of lipid and ion permeation"

Teaching Assistantship

- Spring, 2023 **Course TA & Guest Lecture & Host of workshops**, CHEM585 Statistical Mechanics. Lecture title: "Introduction of Molecular Mechanics and its Biophysical Applications"
- Fall, 2021 **Lab TA**, General Chemistry Lab

Industry Experience

- 2019 – 2020 **Macro-molecular drug developer**, XtalPi Inc. *Duty*: Antibody developability prediction, Antibody database construction & Rosetta-based peptide drug development

Service

- 2023 **Biophysical J**, Reviewer.
- 2022 **Alumni Networking Symposium organization committee**, Chemistry-Biology Interface.