Zhuoran Long

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Current Position

Yale University (Since 2022) New Haven, CT
Postdoc Associate, Chemistry Department
Advisor: Victor S. Batista

Education

New York University (2015 – 2022) New York, NY
Graduate School of Arts and Science, Chemistry Department
Ph.D. in Chemistry
Advisor: Mark E. Tuckerman

Peking University (2011 – 2015) Beijing, China
Yuanpei College
B.S. in Chemistry
Advisor: Yi Qin Gao

Publications

Z. Long, M. E. Tuckerman, "Hydroxide Diffusion in Functionalized Cylindrical Nanopores as Idealized Models of Anion Exchange Membrane Environments: an Ab Initio Molecular Dynamics Study", **2022**, Manuscript submitted.

Z. Long, A. O. Atsango, J. A. Napoli, T. E. Markland, M. E. Tuckerman, "Elucidating the Proton Transport Pathways in Liquid Imidazole with First-Principles Molecular Dynamics", *J. Phys. Chem. Lett.*, **2020**, *11*, 615.

Y. Zhang, D. Poe, L. Heroux, H. Squire, B. W. Doherty, **Z. Long**, M. D. Dadmun, B. E. Gurkan, M. E. Tuckerman, E. J. Maginn, "Liquid Structure and Transport Properties of the Deep Eutectic Solvent Ethaline", *J. Phys. Chem. B*, **2020**, *124*, 5251.

T. Zelovich, **Z. Long**, M. Hickner, S. J. Paddison, C. Bae, M. E. Tuckerman, "Ab initio molecular dynamics study of hydroxide diffusion mechanisms in nanoconfined structural mimics of anion exchange membranes", *J. Phys. Chem. C*, **2019**, *123*, 4638.

X. Cai, W. J. Xie, Y. Yang, **Z. Long**, J. Zhang, Z. Qiao, L. Yang, Y. Q. Gao, "Structure of water confined between two parallel graphene plates", *J. Chem. Phys.*, **2019**, *150*, 124703.

X. Che, X. X. Du, X. Cai, J. Zhang, W. J. Xie, **Z. Long**, Z. Y. Ye, H. Zhang, L. Yang, X. D. Su, Y. Q. Gao, "Single mutations reshape the structural correlation network of the DMXAA–human STING complex", *J. Phys. Chem. B*, **2017**, *121*, 2073.

Projects

New York University, GSAS Chemistry
Proton Transport in Liquid Imidazole

- Liquid imidazole system and an excess proton simulated with *ab initio* molecular dynamics (AIMD) and multi-time stepping scheme.
- Discovered that the protonated imidazole (imidazolium) transported along a dynamic chain of imidazole molecules connected by hydrogen bonds.
- Obtained 3 separated timescales of imidazolium transport: sub-picosecond for local proton transfer within a hydrogen bond; picosecond for imidazolium migration along the hydrogen-bonded chain; ~30 ps for chain component exchange with hydrogen bond dynamics.
- Revealed that size distributions of the hydrogen-bonded imidazole chains follow a simple chemical equilibrium.

Hydroxide Transport in Anion Exchange Membrane (AEM) Model Systems

- Constructed model systems of nanoconfined hydroxide aqueous solutions in graphane nanotube (GN) with tethered organic ammonium cations to mimic local AEM morphology.
- Observed that solution phases were organized as cylindrical layers inside the confinement.
- Discovered that the GN confinement affected hydroxide proton transfer by preferentially aligning the hydroxide along the radial direction, which further resulted in a dangling hydrogen on the proton-donating water.
- Revealed that the hydroxide transport was dominated by structural diffusion (Grotthuss mechanism) in these AEM model systems.
- Revealed that the hydroxide transport was hindered by hydroxide-cation binding.

Fractional Behavior of Molecule Dynamics

- Composed a Python script for non-liner fitting with Mittag-Leffler function, which was the solution to fractional kinetic equations.
- Applied to the proton transport in liquid imidazole where the imidazolium exhibited a possible sub-diffusion feature.
- Applied to the rotational relaxations of a deep eutectic solvent system. Two separated timescales were obtained, indicating two different underlying physics processes.

Acidic Dissociation of $H_2PO_4^-$

- Constructed and simulated $H_2PO_4^-$ – OH^- aqueous solution systems to study the slow acidic dissociation of $H_2PO_4^-$ observed in NMR experiments.
- Revealed that $H_2PO_4^-$ – OH^- reaction was controlled by hydroxide diffusion.
- Discovered that the reaction could happen with a direct proton transfer from $H_2PO_4^-$ to OH^- in a contact ion pair, or a proton transfer relayed by a water molecule in a solvent-separated ion pair.
- Applied a random walk (free diffusion) model in the spherical coordinate and a kinetics model of diffusion-controlled reaction with steady-state assumption to calculate the reaction rate

Peking University

Cellulose Dissolution in NaOH Solutions under Low Temperature

- Constructed systems of cellulose in NaOH solutions and simulated with classical molecular dynamics.
- Applied Two-Phase Thermodynamics (2PT) model to analyze the simulation trajectories, in which the partition function was constructed as the summation of a gas-like part and a solid-like part for entropy calculation. The C++ application code was also applied later to a biomolecular system (STING complex) and a confined water system.