Mary Hongying Cheng

Research Assistant Professor, Department of Chemistry, University of Pittsburgh, PA 15260
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EDUCATION

Rensselaer Polytechnic Institute, **Troy, NY**
Ph.D. Chemical Engineering, Overall GPA: 3.92/4.0 January 2002

Clarkson University, Potsdam, NY
M. S. Chemical Engineering, Overall GPA: 3.83/4.0 May 1997

Tsinghua University, Beijing, P.R. China
B. S. Chemical Engineering, Overall GPA: 3.80/4.0 May 1992

RESEARCH INTEREST

Structural biology, medicinal chemistry, membrane protein channels, effects of drugs on protein receptors, biological and polymer physics, structure-based drug design

RESEARCH EXPERIENCE

Research Assistant Professor May 2008 ~ present
Research Associate May 2003 ~ April 2008
Department of Chemistry, university of Pittsburgh

Drug modulation mechanisms in membrane proteins

- Investigate intravenous anesthetic propofol binding to pentameric ligand-gated ion channels (pLGICs): understanding anesthetic inhibition mechanism in cation-selective ligand-gated ion channels.
- Explored both volatile and intravenous anesthetics binding to pLGICs: identified binding pockets, calculated anesthetic binding energy and investigated the anesthetic modulation mechanism.
- Investigated nicotine binding to neuronal α4β2 nicotinic acetylcholine receptor (nAChR) to understand the channel gating mechanism.
- Identified an intra-subunit binding pocket for ethanol binding to glycine receptor (GlyR) using molecular dynamics (MD): understanding anesthetic potentiation mechanism in anion-selective ligand-gated ion channels.

Ligand-gated ion channels

- Calculated ion permeation characteristics in an open α4β2 nAChR.
- Constructed the glycine receptor channels (GlyRs) using homology modeling and MD and revealed characteristics of channel under three different states: resting, desensitized and open.
- Developed a hybrid Molecular dynamics (MD)/Brownian dynamics (BD) approach to investigate ion permeation and anesthetic halothane effects on pentameric ligand-gated ion channels.

Voltage-gated ClC transporter/channel

- Investigate Cl^-/water transport through eukaryotic CmClC transporter using molecular dynamics.
- Studied a discrete state modeling of ion permeation characteristics in ClC-like channels.
- Simulated the electrostatic control and chloride regulation of the fast gating in chloride channels.

Gape junction Claudin-2 channel

- Build up a numerical model to estimate the relative permeability of claudin-2 channel to different alkali metal cations.
- Investigated inhibition of paracellular Na conductance by calcium and other polyvalent cations using Brownian dynamics.

Lipid-lipid and lipid-protein interactions

- Investigated cholesterol-modified ternary lipid bilayer for functional nicotinic acetylcholine receptor using molecular dynamics simulations.

- Studied lipid-lipid interactions in POPC-POPA-cholesterol ternary lipids and POPE-POPG binary bacterial membrane.

Research Associate February 2002 ~ April 2003
Department of the Chemical and Petroleum Engineering, University of Pittsburgh

- Developed a multi-scale simulation technique to investigate reactive blending and interfacial growth.
- Simulated diblock phase ordering at the presence of preferentially-coated nano rods and spheres.
- Calculated polymer/clay interactions and morphologies using Self Consistent Field theory.

Research Assistant August 1997 ~ January 2002
Department of Chemical and Biological Engineering, Rensselaer Polytechnic Institute, Troy, NY

- Designed experiments to investigate ripening mechanisms in polymer blends on a mezo-scale.
- Performed Monte Carlo simulation of Brownian coalescence and hydrodynamic simulation of spinodal decomposition in polymer blends.
- Made polymer blends PS/PB and PS/PB/PS-PB copolymer using compositional quenching.
- Investigated morphology and particle size distribution in polymer blends using TEM.
- Developed numerical simulation of nonlinear diffusion with concentration driven flows in miscible polymer blends.

Research Assistant August 1995 ~ July 1997
Department of Chemical Engineering, Clarkson University, Potsdam, NY

- Designed and installed experiment to study polymeric extrusion process.
- Developed a three-dimensional numerical simulation for the flow and heat transfer inside the extruder for plastics.

TEACHING EXPERIENCE

Teaching Assistant August 1998 ~ May 2000
Department of Chemical and Biological Engineering, Rensselaer Polytechnic Institute, Troy, NY

- Instructed undergraduates in the senior lab

WORK EXPERIENCE

Process Design and Development Engineer August 1992 ~ May 1995
Chengdu Silicone Research Center, Chengdu, P. R. China

- Conducted organic synthesis, completed separation tower design and the Process & Instrumentation Design of "Synthesis of Silane Coupling Agent" using Computer-aided Design.
- Calculated heat/material balance of "Synthesis of High Temperature Vulcanite", and independently completed the Process & Instrumentation Design using Computer-aided Design

PUBLICATIONS

1. **Mary H. Cheng**, Lu Liu, David Mowrey, Troy Wymore, Yan Xu, and Pei Tang," Symmetry of Anesthetic Binding Sites in the Pentameric Ligand-Gated Ion Channel GLIC Affects Transition of Channel Conformations" submitted (2011).
2. **Mary H. Cheng**, and Rob D. Coalson, "Molecular dynamics investigation of chloride and water transport through a eukaryotic ClC transporter", submitted (2011).
3. Rob D. Coalson and **Mary H. Cheng**," Discrete-State Representation of Ion Permeation Coupled to Fast Gating in a Model of CLC-chloride Channels: Analytic Estimation of the State-to-State Rate Constants", *J*. Phys*. Chem. A*, *115*, 9633–9642**.** (2011).
4. **Mary H. Cheng**, Coalson RD, and Tang P. Molecular dynamics and Brownian dynamics investigation of ion permeation and anesthetic halothane effects on a proton−gated ion channel. *J Am Chem Soc;* 132, 16442-9 (2010).

5. Qiang Chen, **Mary H. Cheng**, Xu Yan, and Tang P. Anesthetic Binding in a Pentameric Ligand-gated Ion Channel: GLIC, *Biophy. J*, 99, 1801-1809 (2010).
6. Yu A, **Mary H. Cheng**, Coalson RD: Inhibition of paracellular Na conductance by calcium and other polyvalent cations through the proximal tubule tight junction protein claudin-2, *J. Biol. Chem*. 285, 37060-9 (2010).
7. Rob D. Coalson, and **Mary H. Cheng**, "Discrete-State Representation of Ion Permeation Coupled to Fast Gating in a Model of ClC-chloride Channels: Comparison to Multi-ion Continuous Space Brownian Dynamics Simulations", *J. Phys. Chem. B* 114, 1424-1433 (2010).
8. **Mary H. Cheng**, Yan Xu and Pei Tang，"Anionic Lipid and Cholesterol Interactions with α4β2 nAChR: Insights from MD Simulations", *J. Phys. Chem. B*, 113 , 6964–6970 (2009).
9. A. Yu, **Mary H. Cheng**, S. Angelow, D. Günzel, S. Kanzawa, E. Schneeberger, M. Fromm, Rob D. Coalson, "Molecular basis for cation selectivity in claudin-2-based paracellular pores: Identification of an electrostatic interaction site", *Journal of General Physiology*, 133, 111-127 (2009).
10. **Mary H. Cheng,** RD Coalson, M.Cascio, and M. Kurnikova, "Computational prediction of ion permeation characteristics in the glycine receptor modified by photo-sensitive compounds", *J. Comput. Aided Mol. Des.* 22, 563-570, (2008)
11. E. Haddadian, **Mary H. Cheng**, RD Coalson, Yan Xu, and Pei Tang, "In silico models for the human α4β2 nicotinic actytcoline receptor", *Journal of Physical Chemistry B*, 112, 13981-90 (2008).
12. **Mary H. Cheng,** Rob D. Coalson, and Michael Cascio "Molecular dynamics simulations of binding ethanol to the GlyR transmembrane domain: Implications of channel potentiation mechanism", *Proteins: Structure, Function and Bioinformatics,* 71, 972-981 (2008).
13. **Mary H. Cheng,** L. Liu, A. Saladino, Yan Xu, and Pei Tang "Ternary membrane mixture for functional nAChR", *Journal of Physical Chemistry B*, 111, 14186-14192 (2007).
14. **Mary H. Cheng,** M. Cascio, and Rob D. Coalson, "Homology Modeling and Molecular Dynamics Simulation of the Glycine α1 Receptor Revealed Different States of Channel", *Proteins*: *Structure, Function and Bioinformatics*, 68. 581-593 (2007).
15. **Mary H. Cheng**, A. Mamonov, W. Duke and Rob D. Coalson, "Modeling of electrostatic control and chloride regulation of the fast gating in the ClC-0 chloride channels", *Journal of Physical Chemistry B*, 111, 5956-5965 (2007).
16. **Mary H. Cheng,** Michael Cascio, and Rob D. Coalson, "Theoretical Studies of the Transmembrane Segment of the Glycine Receptor: Models of the Open Pore Structure and Current-Voltage Characteristics", featured cover in *Biophysical Journal*, 89. 1669-1680 (2005).
17. **Mary H. Cheng**, and Rob D. Coalson, "An accurate and efficient empirical approach to calculate the dielectric self energy and ion-ion interaction in biological ion channels", *Journal of Physical Chemistry B*., 109. 488-498 (2005)
18. **Mary H. Cheng** and E.B. Nauman**, "**Phase Ripening in Particulate Binary Polymer Blends", *Journal of Polymer Science Part B: Polymer Physics*, 42, 603-612 (2004).
19. **Mary H. Cheng**, A.C. Balazes, C. Yeung, and V. Ginzburg, "Modeling Reactive Compatibilization of a Binary Blend with Interacting Particles", *J. Chem. Phys.* 118 9044 – 9052 (2003).
20. **Mary H. Cheng** and E.B. Nauman, "Non-linear Diffusion with Concentration Driven Flow in Miscible Systems", *Polymer* 44, 6707-6712 (2003).
21. Nauman, E. B. and **Mary H. Cheng**, "Application of Cahn-Hilliard equation to miscible systems", *A.I.A.A*, 2002-886, 1-5 (2002).
22. Campbell GA, Wang C, **Cheng H**, Bullwinkel M, te-Riele MA," Investigation of flow rate and viscous dissipation in a single screw pump-extruder", *Intl. Poly. Proc. 16 (4)*, 323-333 (2001).

INVITED TALK

Mary Hongying Cheng, "Modeling Ligand-gated ion Channels: Structure, Function, and Modulation Mechanism by Anesthetics", Rush University Medical Center, Chicago, June 13, 2011.

Mary Hongying Cheng, "Modeling Ion Channels: Structure, Function, and Modulation Mechanism by Membrane Lipids", St. Jude Children's Research Hospital, Memphis, March 4, 2009.

Mary Hongying Cheng, "Numerical modeling of fast gate-coupled ion permeation in ClC channels", American Physical Society meeting, Pittsburgh, March, 2009

Mary Hongying Cheng, "Modeling Neurotransmitter-gated Ion Channels", University of California Irvine, Irvine, February 18, 2008.

Mary Hongying Cheng, "Numerical Modeling of Membrane Protein Channels", Georgia State University, Atlanta, January 21, 2008.

Mary Hongying Cheng, "Glycine receptor transmembrane domain: structures, channel potentiation mechanism and ion permeation kinetics", American Chemistry Society meeting, Boston, August 21, 2007.

SELECTED PRESENTATIONS and POSTERS

1. **Mary H. Cheng**, Yan Xu, Rob D Coalson, and Pei Tang, "Molecular Dynamics Investigation of Anesthetic Halothane Interactions with the Proton-Gated Ion Channel GLIC", Biophysical society meeting, March, 2010.
2. **Mary H. Cheng**, E. Haddadian, Yan Xu, and Pei Tang, "Interactions between POPA and α4β2 nAChR: Insights from MD simulations", Biophysical society meeting, March, 2009.
3. **Mary H. Cheng,** Rob D. Coalson, and Michael Cascio "Molecular dynamics simulations of binding ethanol to the GlyR transmembrane domain: Implications of channel potentiation mechanism", Biophysical society meeting, March 5, 2007.
4. **Mary H. Cheng,** M. Cascio, and Rob D. Coalson, "Homology Modeling and Molecular Dynamics Simulation of the Glycine α1 Receptor Revealed Different States of Channel", Biophysical society meeting, March 5, 2007.

GRANTS and AWARDS

Outstanding Student Award of Tsinghua University, offered only to the top 10 %, 1988-1992.

1. **Mary H. Cheng** and Rob D Coalson, "Large-scale molecular dynamics and Brownian dynamics investigation of ion permeation through the ligand-gated ion channel". Computational Grant TG-MCB100061.
2. **Mary H. Cheng** and Rob D Coalson, "Large-scale molecular dynamics and discrete-state modeling of Cl^- transport through CmCLC transporter". Computational Grant TG-MCB050030N.

COMPUTER SKILLS

Language: C, C++, FORTRAN, Java, SQL, Perl, TCL, HTML
Software: Matlab, NAMD, VMD, MODELLER, CHARMM, AMBER, PROCHECK, AUTODOCK
Simulation: Molecular Dynamics, QM/MM, Dynamic Monte Carlo, Brownian Dynamics, Homology modeling, Discrete State Modeling, Hydrodynamics
Operation systems: Linux/unix, Windows