

## Hwan Kyu Lee, Ph.D.

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### PERSONAL INFORMATION

Date of Birth      September 10, 1976  
Citizenship      South Korea (U.S. Permanent Resident)

### EDUCATION

- 5/2004 ~ 2/2007    **Ph.D. University of Michigan (Ann Arbor), Biomedical Engineering**  
Dissertation title: Molecular dynamics studies of peptide, nanoparticle, and lipid interactions using multiscale simulations.  
**Advisor: Prof. Ronald G. Larson in Chemical Eng. (National Academy of Engineering)**
- 9/2002 ~ 4/2004    M.S. University of Michigan (Ann Arbor), Biomedical Engineering  
Coursework: Biophysical chemistry, Systems biology, Bioinformatics and gene expression, Chemoinformatics, Cell Biology, Biostatistics, Physiology, Biomaterials, Tissue engineering
- 3/1995 ~ 2/2002    B.S. Chung-ang University (Seoul, South Korea), Chemical Engineering  
Coursework: Thermodynamics, Reaction engineering, Fluid mechanics, Heat & Mass transfer, Physical chemistry, Process control, Organic chemistry, Biochemistry, Biochemical engineering

### EMPLOYMENT

- 3/2007 ~ present    **Research Fellow, NHLBI, National Institutes of Health, Bethesda, MD**  
**Advisor: Dr. Richard W. Pastor**
- 9/2003 ~ 2/2007    Graduate Research Assistant, Biomedical Engineering, University of Michigan, Ann Arbor, MI
- 11/1997 ~ 1/2000    Korean Army (Engineering battalion), Yang-gu, Kangwon-do

### RESEARCH INTERESTS

1. Computational Biophysics and Nanoscience: multiscale molecular dynamics simulations  
Goal: rational design of synthetic peptides, nanoparticles, and drug complexes
  - Structure and dynamics of peptides interacting with monolayers and micelles: the effect of individual amino acids on conformation of lung-surfactant, BAR, and coiled-coil peptides
  - Nanoparticle-induced membrane curvature and pore formation: the effects of dendrimer charge density, size, concentration and molecular shape, rationalized by electrostatic interactions
  - Polymer physics in water and on various surfaces: the transport of polymers through membrane nanopores; the transition from ideal to swollen-coil behavior in water; the transition between mushroom and brush on surfaces
  - Self-assembly of polymer-conjugated vesicles, bicelles, and micelles: polymer concentration dependence of phase behaviors
  - Parameterization of all-atom and coarse-grained models for simulations described above
2. Biophysical experiments: circular dichroism spectroscopy & single-channel current recording in nanopore
  - Salt concentration dependence on interactions between dendrimer and  $\alpha$ -hemolysin channel

## TEACHING EXPERIENCE

Summer/2009      National Institutes of Health, Bethesda, MD  
- Advised an intern to study fundamentals of molecular dynamics simulations and simulate polymers grafted on various surfaces

## PUBLICATIONS (2005/12 ~ Current) (\*corresponding author)

1. **Lee H**, Kandasamy SK, and Larson RG, Molecular dynamics simulations of the anchoring and tilting of the lung-surfactant peptide SP-B<sub>1-25</sub> in palmitic acid monolayers. *Biophysical J.*, **2005**, 89:3807-3821
2. **Lee H**, Baker JR, and Larson RG, Molecular dynamics studies of the size, shape, and internal structure of 0% and 90%-acetylated G5 PAMAM dendrimers in water and methanol. *J. Physical Chemistry B*, **2006**, 110:4014-4019
3. Sayer JA, Otto EA, O'toole JF, Nurnberg G, Kennedy MA, Becker C, Hennies HC, Helou J, Attanasio M, Fausett BV, Utsch B, Khanna H, Liu Y, **Lee H**, Larson RG, and Hildebrandt F et al., The centrosomal protein nephrocystin-6 is mutated in Joubert syndrome and activates transcription factor ATF4. *Nature Genetics*, **2006**, 38:674-681
4. **Lee H**, and Larson RG, Molecular dynamics simulations of PAMAM dendrimer-induced pore formation in DPPC bilayers using a coarse grained model. *J. Physical Chemistry B.*, **2006**, 110:18204-18211
5. **Lee H**, and Larson RG, Prediction of the stability of coiled coils using molecular dynamics simulations. *Molecular Simulation*, **2007**, 33:463-473
6. **Lee H\***, and Larson RG, Coarse-grained molecular dynamics studies of the concentration and size dependence of fifth- and seventh-generation PAMAM dendrimers on pore formation in DMPC bilayer. *J. Physical Chemistry B.*, **2008**, 112:7778-7784
7. **Lee H\***, and Larson RG, Lipid bilayer curvature and pore formation induced by charged linear polymers and dendrimers: the effect of molecular shape. *J. Physical Chemistry B.*, **2008**, 112:12279-12285
8. **Lee H**, Venable RM, MacKerell AD, and Pastor RW, Molecular dynamics studies of polyethylene oxide and polyethylene glycol: hydrodynamic radius and shape anisotropy. *Biophysical J.*, **2008**, 95:1590-1599
9. Low C, Weininger U, **Lee H**, Schweimer K, Neundorf I, Beck-Sickinger AG, Pastor RW, and Balbach J, Structure and dynamics of helix-0 of the N-BAR domain in lipid micelles and bilayers. *Biophysical J.*, **2008**, 95:4315-4323
10. **Lee H\***, and Larson RG, Multiscale modeling of dendrimers and their interactions with bilayers and polyelectrolytes. *Molecules*, **2009**, 14:423-438
11. **Lee H**, de Vries AH, Marrink SJ and Pastor RW, A coarse-grained model for polyethylene oxide and polyethylene glycol: conformation and hydrodynamics. *J. Physical Chemistry B.*, **2009**, 113:13186-13194
12. **Lee H**, and Pastor RW, Polyethylene glycol concentration dependence of phase behaviors of self-assembled vesicles, bicelles, and micelles. *J. Am. Chem. Soc. In preparation.*

## CHAPTERS IN BOOKS

Kandasamy SK, Lee H, and Larson RG, "Computer simulations of dendrimers". Invited chapter in the book "Dendrimer-based nanomedicine" edited by James Baker, Jr., Istvan Majoros., Pan Stanford publishing, 2008

## PRESENTATIONS

1. Lee H, Kandasamy SK, and Larson RG, Molecular dynamics simulations of the anchoring and tilting of the lung-surfactant peptide SP-B<sub>1-25</sub> in palmitic acid monolayers. *Platform-talk, 2005 Biophysical Society Meeting, CA*
2. Lee H, and Larson RG, Can molecular dynamics simulations predict the stability and conformation of coiled coil peptides?, *Poster, 2006 Biophysical Society Meeting, UT*
3. Lee H, Kandasamy SK, and Larson RG, Molecular dynamics simulations of PAMAM dendrimer-induced pore formation in DPPC bilayers using a coarse grained model, *Poster, 2006 American Chemical Society Meeting, CA*
4. Lee H, Venable RM, MacKerell AD, and Pastor RW, Molecular dynamics simulations of polyethylene oxide and glycol. *Poster, 2008 Biophysical Society Meeting, CA*
5. Lee H and Larson RG, Lipid Bilayer Curvature and Pore Formation Induced by Charged Linear Polymers and Dendrimers: The Effects of Charge Density, Concentration, Molecular Size and Shape, *2008 AIChE annual meeting, PA*

## MEMBERSHIP

Biophysical Society, American Chemical Society

## REFEREE EXPERIENCE

Journal of the American Chemical Society, Journal of Computational Chemistry, Journal of Physical Chemistry B, Macromolecules

## GRANT REVIEW

Division for Chemical Sciences of the Netherlands Organization for Scientific Research (NWO)

## COMPUTER SKILLS

Tools                   CHARMM, GROMACS, AMBER, Swiss-PdbViewer, Cerius2 (Molecular dynamics simulation); Cellerator, Banjo, NetLogo (Systems biology); SMILES, SMARTS, Molinspiration, CACTVS, GIF generator (Chemoinformatics); SPOTFIRE (Bioinformatics statistical analysis); LabView; HYSYS (Process simulation); Excel (Spreadsheets)

Languages/OS       C/C++, Python, Tcl, Mathematica, MATLAB, Linux, Unix, Mac, Windows

## EXPERIMENTAL SKILLS

Single-channel current recording in planar lipid bilayer, Circular dichroism spectroscopy, PCR, Bioanalyzer, Epifluorescence microscopy (Axiovert 135TV, Zeiss), Ion-exchange chromatography, Spectrophotometer, Ultrasonic dismembrator, Ultracentrifuge, SDS-electrophoresis

## AWARDS

2/2001                   Merit-based Scholarship, Chung-ang University

## REFERENCES

Ronald G. Larson       Chemical Engineering and Biomedical Engineering, University of Michigan, Ann Arbor, MI (734) 936-0772, rlarson@umich.edu

Richard W. Pastor     Lab. of Computational Biology, NHLBI, National Institutes of Health, Bethesda, MD (301) 435-2035, pastorr@nhlbi.nih.gov

Siewert-Jan Marrink   Groningen Biomolecular Sciences and Biotechnology Institute and Zernike Institute for Advanced Materials, University of Groningen, Netherlands +31 (0) 50-363-4457, s.j.marrink@rug.nl