Curriculum Vitae

Name	:	Wonpil Im	Date of Birth	:	March 10, 1970
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I. EDUCATION

06/2002	–	Present	NSF CTBP (Center for Theoretical Biological Physics) Fellow Postdoctral Associate in the group of Prof. Charles Brooks, The Scripps Research Institute, La Jolla
02/1997	–	05/2002	Ph. D. in Biochemistry Weill Medical College of Cornell University, New York Thesis Supervisor: Prof. Benoit Roux
(02/1997	–	05/2000	in Chemistry, University of Montreal, Montreal)
03/1994	–	02/1996	M. Sc. in Chemistry, Hanyang University, Seoul Thesis Supervisor: Prof. Youngdo Won
03/1990	–	02/1994	B. Sc. in Chemistry, Hanyang University, Seoul

II. EXPERIENCE

1. Postdoctoral Research Experience
   - Development of Generalized Born Model (GBSW module in CHARMM).
   - Folding, assembly, and modeling of membrane peptides/proteins.
   - Membrane insertion and interfacial folding of synthetic peptides (WALP and TMX).
   - Structure refinement of proteins with implicit solvent models.
   - Molecular dynamics simulations with implicit solvent models for proteins and DNA.

2. Doctoral Research Experience
   - Molecular dynamics simulations of aqueous salt solutions.
   - Molecular dynamics simulations of the membrane-protein system (OmpF porin).
   - Grand Canonical Monte Carlo - Brownian Dynamics (GCMC/BD) simulations of ion permeations through the porin (OmpF, PhoE, OmpK36, and mutants of OmpF).
   - PNP (Poisson-Nernst-Planck) solver and its applications to porins.
   - Generalized Solvation Boundary Potentials (GSBP).
   - Electrostatic solvation forces based on the Poisson-Boltzmann equation.
   - Development of CHARMM source code (PBEQ/GSBP module).

3. Pre-doctoral Research Experience
   - Molecular dynamics simulations of liquid systems (normal alkanes and acetonitrile).
   - Parameterization of acetonitrile.
   - Potential of mean force (PMF) calculations for the anion pair formation of acetonitrile.
   - Development of CHARMM source code (CRYSTAL module).

4. Teaching experience
   - Aug. 9 2004 — Aug. 20 2004 2004 CTBP Summer Workshop, UCSD
   - Jan. 2002 — April 2002 Teaching Assistant in Department of Biochemistry Weill Medical College of Cornell University
   - March 1995 — Feb. 1996 Teaching Assistant in Department of Chemistry Hanyang University

5. Honors
   - 2002 Graduate School Scholarship Award of Excellence (May, 2002)

III. REFEREES

1. Professor Charles L. Brooks, III
   Department of Molecular Biology (TPC6), The Scripps Research Institute
   10550 North Torrey Pines Rd, La Jolla, CA 92037
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2. Professor Benoit Roux
   Department of Biochemistry, Weill Medical College of Cornell University
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3. Professor David A. Case
   Department of Molecular Biology (TPC15), The Scripps Research Institute
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4. Professor Shin-Ho Chung
   Biophysics Group, Department of Physics, The Australian National University
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5. Professor Olaf Sparre Andersen
   Department of Physiology and Biophysics, Weill Medical College of Cornell University
   1300 York Avenue, New York, NY 10021
   Tel.~: (212) 774-2289
   Email: sparre@med.cornell.edu

IV. INVITED TALKS

1. Insertion and Folding Mechanism of Membrane Peptides and Proteins Studied by Molecular Simulation, The Protein Society's 18th Annual Symposium, San Diego, USA (2004)
2. Atoms in Motion, 3rd Symposium of Korean-American Scientists and Engineers Association at San Diego Chapter (KSEA-SD), San Diego, USA (2004)
3. De Novo Folding of Membrane Proteins, Theory and Applications of Computational Chemistry, Gyeongju, KOREA (2004)
4. An Implicit Membrane Generalized Born Theory for the Study of Structure, Stability, and Interactions of Membrane Proteins. 5th Canadian Computational Chemistry Conference, Toronto, CANADA (2003)
5. The Role of Electrostatics in Ion Permeation and Selectivity of Biological Membrane Channels. Department of Chemistry, Hanyang University, Seoul, KOREA (2002)
6. Ion Permeation and Selectivity of OmpF Porin from Eschericha coli: Theoretical Studies using Molecular Dynamics, Brownian Dynamics, and the Electrodiffusion Theory. 46th Annual Biophysical Society Meeting, San Francisco, USA (2002)
7. Ion Permeation and Selectivity of OmpF Porin from Eschericha coli: Theoretical Studies using Molecular Dynamics, Brownian Dynamics, and the Electrodiffusion Theory. Laboratory of Chemical Physics, NIDDK, National Institutes of Health, USA (2001)

V. REFEREED JOURNALS

1. **W. Im**, J. Chen, and C.L. Brooks III
   Performance of a Generalized Born / Nonpolar Solvation Model with a Simple Switching Function. in preparation (2004).
2. **W. Im** and C.L. Brooks III
   Interfacial Folding and Membrane Insertion: A Molecular Dynamics Study with Synthetic Peptides. submitted (2004).
3. J. Chen, H. Won, **W. Im**, H.J. Dyson and C.L. Brooks III
   Generation of Native-like Models from limited NMR data. *J. Biomolec. NMR* in press (2004).
4. J. Chen, **W. Im**, and C.L. Brooks III
   Refinement of NMR Structure Using Implicit Solvent and Advanced Sampling Techniques. *J. Am. Chem. Soc.* in press (2004).
5. S.Y. Noskov, **W. Im**, and B. Roux
   Ion Permeation through the □-Hemolysin Channel: Theoretical Studies based on Brownian Dynamics and Poisson-Nernst-Plank Electrodiffusion Theory. *Biophys. J.* 87:2299-2309 (2004).
6. B. Roux, T. Allen, S. Berneche, and **W. Im**
   Theoretical and Computational Models of Ion Channels. *Q. Rev. Biophys.* 37:15-103 (2004).
7. **W. Im** and C.L. Brooks III
   De Novo Folding of Membrane Proteins: An Exploration of the Structure and NMR Properties of the fd Coat Protein. *J. Mol. Biol.* 337:513-519 (2004).

8. M. Feig, **W. Im**, and C.L. Brooks, III
   Implicit Solvation Based on Generalized Born Theory in Different Dielectric Environment. *J. Chem. Phys.* 120:903-911 (2004).
9. M. Feig, A. Onufriev1, M.S. Lee, **W. Im**, D.A. Case, and C.L. Brooks, III
   Performance Comparison of Generalized Born and Poisson Methods in the Calculation of Electrostatic Solvation Energies for Protein Structures. *J. Comput. Chem.* 25:265-284 (2004).
10. **W. Im**, M. Feig, and C.L. Brooks III
    An Implicit Membrane Generalized Born Theory for the Study of Structure, Stability, and Interactions of Membrane Proteins. *Biophys. J.* 85:2900-2918 (2003).
11. **W. Im**, M.S. Lee, and C.L. Brooks III
    Generalized Born Model with a Simple Smoothing Function. *J. Comput. Chem.* 24:1691-1702 (2003).
12. N.K. Banavali, **W. Im**, and B. Roux
    Electrostatic Free Energy Calculations using the Generalized Solvent Boundary Potential Method. *J. Chem. Phys.* 117:7381-7388 (2002).
13. **W. Im** and B. Roux
    Ion Permeation and Selectivity of OmpF Porin: A Theoretical Study Based on Molecular Dynamics, Brownian Dynamics, and Continuum Electrodiffusion Theory. *J. Mol. Biol.* 322:851-869 (2002).
14. **W. Im** and B. Roux
    Ions and Counterions in a Biological Channel: A Molecular Dynamics Simulation of OmpF Porin from Escherichia coli in an Explicit Membrane with 1 M KCl Aqueous Salt Solution. *J. Mol. Biol.* 319:1177-1197 (2002).
15. A. Philippsen, **W. Im**, A. Engel, T. Schirmer, B. Roux, and D.J. Muller
    Imaging the Electrostatic Potential of Transmembrane Channels: Atomic Probe Microscopy of OmpF Porin. *Biophys. J.* 82:1667-1676 (2002).
16. **W. Im** and B. Roux
    Brownian Dynamics Simulations of Ions Channels: A General Treatment of the Electrostatic Reaction Field for Molecular Pores of Arbitrary Geometry. *J. Chem. Phys.* 115:4850-4861 (2001)
17. **W. Im**, S. Berneche, and B. Roux
    Generalized Solvent Boundary Potentials for Computer Simulations. *J. Chem. Phys.* 114:2924-2937 (2001).
18. B. Roux, S. Berneche and **W. Im**
    Ion Channels, Permeation, and Electrostatics: Insight into the Function of KcsA. *Biochemistry* 39:13295-13306 (2000).
19. **W. Im**, S. Seefeld and B. Roux
    Grand Canonical Monte Carlo - Brownian Dynamics Algorithm for Simulating Ion Channels. *Biophys. J.* 79:788-801 (2000).
20. M. Nina, **W. Im**, and B. Roux
    Optimized Atomic Radii for Protein Continuum Electrostatics Solvation Forces. Biophys. Chem. 78:89-96 (1999).

21. **W. Im**, D. Beglov, and B. Roux
    Continuum Solvation Model: Computation of Electrostatic Forces from Numerical Solutions to the Poisson-Boltzmann Equation. *Comput. Phys. Comm.* 111:59-75 (1998).
22. **W. Im** and Y. Won
    Molecular Dynamics Simulation on Thermodynamic and Structural Properties of Liquid Hydrocarbons : Normal Alkanes. *bull. Korean Chem. Soc.* 15:852-856 (1994).

VI. BOOK CHAPTERS & THESIS

1. **W. Im** and C.L. Brooks III
   Structure prediction of membrane proteins. *In* Computational Methods for Protein Structure Prediction and Modeling, Springer-Verlag Press, Ying Xu , Dong Xu, and Jie Liang Eds. in preparation (2005)

2. B. Roux, D. Beglov, and **W. Im**
   Generalized Solvent Boundary Potentials for Computer Simulations. *In* Treatments of electrostatics interactions in computer simulations of condensed media, Santa Fe Workshop, L.R. Pratt and G. Hummer Eds. 492:473-491 (1999).

3. **W. Im**
   The Role of Electrostatics in Ion Permeation and Selectivity of Biological Membrane Channels. Ph.D. Thesis. Cornell University. (2002)

4. **W. Im**
   Molecular Dynamics Simulation on Thermodynamic, Structural, and Dynamic Properties of Liquid Alkanes and Liquid Acetonitrile. M. Sc. Thesis}. Hanyang University. (1996)