

Curriculum Vitae

Name Wonpil Im
Sex Male
Date of Birth March 10, 1970
Nationality Korean

Email *wonpil@scripps.edu*

Mailing Address Wonpil Im (in Brooks Lab)
Department of Molecular Biology (TPC6)
The Scripps Research Institute
10550 North Torrey Pines Rd
La Jolla, CA 92037

Telephone & (858) 784-8214
Fax Number (858) 784-8688

I. EDUCATION

June 2002 - present Postdoctoral Associate in the Brooks group,
The Scripps Research Institute, La Jolla

Feb. 1997 - May 2002 Ph. D. in Biochemistry,
Weill Medical College of Cornell University, New York

(Feb. 1997 - May 2000 in Chemistry, University of Montreal, Montreal)
Thesis Supervisor : Prof. B. Roux

March 1994 - Feb. 1996 M. Sc. in Chemistry, Hanyang University, Seoul
Thesis Supervisor : Prof. Y. Won

March 1990 - Feb. 1994 B. Sc. in Chemistry, Hanyang University, Seoul

II. EXPERIENCE

1. Postdoctoral Research Experience

- Generalized Born Model (GBSW module in CHARMM).
- Folding, assembly, and modeling of membrane proteins.
- Structure refinement of proteins with implicit solvent models
- Molecular dynamics simulations with implicit solvent models for proteins and DNA (or RNA).

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 (PBFORCE).
- 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

March 1995 - Feb. 1996 Teaching Assistant in Department of Chemistry
Hanyang University

Jan. 2002 - April 2002 Teaching Assistant in Department of Biochemistry
Weill Medical College of Cornell University

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

Tel. : (858) 784-8035

Email: brooks@scripps.edu

2. Professor Benoît Roux

Department of Biochemistry, Weill Medical College of Cornell University

1300 York Avenue, New York, NY 10021

Tel. : (212) 746-6018

Email: benoit.roux@med.cornell.edu

3. 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. 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)
2. The Role of Electrostatics in Ion Permeation and Selectivity of Biological Membrane Channels.
Department of Chemistry, Hanyang University, Seoul, KOREA (2002)
3. Ion Permeation and Selectivity of OmpF Porin from Escherichia coli: Theoretical Studies using Molecular Dynamics, Brownian Dynamics, and the Electrodiffusion Theory.
46th Annual Biophysical Society Meeting, San Francisco, USA (2002)
4. Ion Permeation and Selectivity of OmpF Porin from Escherichia 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** and C.L. Brooks III
de novo Membrane Protein Folding: fd coat Protein and its NMR Properties.
in preparation (2003).
2. B. Roux, T. Allen, S. Bernèche and **W. Im**
Theoretical and Computational Models of Ion Channels.
Q. Rev. Biophys. submitted (2003).
3. M. Feig, **W. Im**, and C.L. Brooks, III
Implicit Solvation Based on Generalized Born Theory in Different Dielectric Environment.
J. Chem. Phys. in press (2003).
4. **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. in press (2003).
5. 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. in press (2003).

6. **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).
7. 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).
8. **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).
9. **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).
10. 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).
11. **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).
12. **W. Im**, S. Bernèche, and B. Roux
Generalized Solvent Boundary Potentials for Computer Simulations.
J. Chem. Phys. 114:2924-2937 (2001).
13. B. Roux, S. Bernèche and **W. Im**
Ion Channels, Permeation, and Electrostatics: Insight into the Function of KcsA.
Biochemistry 39:13295-13306 (2000).
14. **W. Im** and S. Seefeld and B. Roux
A Grand Canonical Monte Carlo - Brownian Dynamics Algorithm for Simulating Ion Channels.
Biophys. J. 79:788-801 (2000).

15. M. Nina, **W. Im**, and B. Roux
Optimized Atomic Radii for Protein Continuum Electrostatics Solvation Forces.
Biophys. Chem. 78:89-96 (1999).
16. **W. Im**, D. Beglov, and B. Roux
Continuum Solvation Model: Computation of Electrostatic Forces from Numerical Solutions to the Poisson-Boltzmann Equation.
Computer Physics Communication 111:59-75 (1998).
17. **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. THESIS AND BOOK CHAPTERS

1. **W. Im**
The Role of Electrostatics in Ion Permeation and Selectivity of Biological Membrane Channels.
Ph.D. Thesis. Cornell University. (2002)
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**
Molecular Dynamics Simulation on Thermodynamic, Structural, and Dynamic Properties of Liquid Alkanes and Liquid Acetonitrile.
M. Sc. Thesis. Hanyang University. (1996)