

## **CURRICULUM VITAE**

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### **EDUCATIONAL/RESEARCH BACKGROUND**

1. Associate professor at Sejong University  
2008. 3 ~ Current
2. Assistant professor at Sejong University  
2006. 9 ~ 2008. 2
3. Research associate at Seoul National University  
2004. 9 ~ 2006. 8
4. Contract assistant professor at Seoul National University  
2000. 9 ~ 2004. 8
5. Visiting Scholar  
IAMS(Institute of Atomic and Molecular Science), Academia Sinica, Tawain,  
2003. 1. 9 ~ 2003. 1. 29 (with prof. Sheng-Hsien Lin)
6. Postdoctoral fellow at University of Utah.  
1997.1 ~ 2000. 8 (with prof. Gregory A. Voth)
7. Postdoctoral fellow at the University of Chicago.  
1996. 9 ~ 1996. 12
8. Ph. D. at the University of Chicago.  
1990. 9 ~ 1996. 8 (Under the guidance of prof. Stuart A. Rice)
9. M.S. Yonsei University, Seoul, Korea (Under the guidance of prof. Ungin Cho)  
1987. 3 ~ 1989. 2
10. B.S. at Yonsei University, Seoul, Korea  
1983. 3 ~ 1987. 2

### **EXTERNAL RESEARCH FUNDING**

1. Research funding for new professor, "Study of quantum phase transition on molecular cluster", 2001. 9 ~ 2002. 8, Korea Research Foundation.
2. Research funding for young scientist, "Theoretical study of complex molecular system: bio-molecules", 2003. 7 ~ 2004. 7 Korea Science Foundation.
3. Research Funding for Basic Science, "Computational study of disease causing proteins", 2007.10. ~ 2009. 9, Korea Science Foundation
4. Research Funding for new scientist, "Computational study of protein association using simple model", 2009.5~2011.4, Korea Science Foundation.

## TEACHING EXPERIENCES

### Teaching Assistant

- General Chemistry, Dept. of Chemistry, Yonsei Univ. Seoul, Korea  
Mar. 1987 – Feb. 1989.
- Physical Chemistry, Dept. of Chemistry, The Univ. of Chicago,  
Apr. 1994 - Jun. 1994.
- Thermodynamics, Dept. of Chemistry, The Univ. of Chicago,  
Nov. 1991 - Jan. 1992, Jan. 1993 - Mar. 1993.
- General Chemistry, Chemistry Department, The Univ. of Chicago,  
Oct. 1990 – Jul. 1991, Apr. 1995 - Jun. 1995.

### Lecture

- General Chemistry, Dept. of Chemistry, Seoul National University,  
(2001.3 ~ 2001.6, 2002.3~2002.6).

### Assistant and Associate professor

- General Chemistry
- Physical Chemistry
- Bio-Physical Chemistry
- Experiments in Physical Chemistry
- Environmental Chemistry

## RESEARCH EXPERIENCE

### Assistant and Associate professor

- Computer simulation/modeling of bio-molecules.
- Aggregation of proteins.
- *Ab initio* electronic structure calculation of organic/bio-molecules.

### Contract assistant professor.

- Computer simulation/modeling of bio-molecules.
- Development of efficient conformational searching scheme of biomolecules.
- *Ab initio* electronic structure calculation of organic/bio-molecules.

### Postdoctoral fellow

- Condensed matter simulations
- Molecular dynamics (MD)/Monte Carlo (MC) simulation
- High energy density matter(HEDM) study (with US Air Force)
- High performance/Large scale parallel computation (with US Air Force)
- Software development
- Quantum/Classical molecular dynamics

### Ph. D.

- Theoretical study of reaction rate and development of alternative reaction rate theory
- Nonlinear dynamics calculations
- Classical trajectory calculations
- Reaction path analysis
- Quantum/Classical correspondence
- Quantum mechanical wave packet propagations, Quantum rate calculations
- Complex scaling to quantum mechanics and dynamical resonance calculations

M. S.

- Theoretical study of chemical laser;

## PUBLICATIONS

1. "Comment on the rate of isomerization in molecules with a symmetric triple well potential", Soonmin Jang, Meishan Zhao and Stuart A. Rice, J. Chem. Phys. 97, 8188 (1992).
2. "Reaction path analysis of the rate of unimolecular isomerization", Soonmin Jang and Stuart A. Rice, J. Chem. Phys. 99, 9585 (1993).
3. "On the classical theory of the rate of isomerization of HCN", Hui Tang, Soonmin Jang, Meishan Zhao and Stuart A. Rice, J. Chem. Phys. 101, 8737 (1994).
4. "Comment on quantum transition state theory", Stuart A. Rice, Soonmin Jang and Meishan Zhao, J. Phys. Chem. 100, 11893 (1996) (Robin M. Hochstrasser Festschrift).
5. "Semiclassical Quantum Unimolecular Reaction Rate Theory Revisited", Soonmin Jang, Meishan Zhao and Stuart A. Rice, Chemical Physics 230, 237-251 (1998).
6. "Intramolecular Energy Transfer in the Isomerization of Cyclobutanone", Hui. Tang, Soonmin. Jang, Meishan Zhao and Stuart A. Rice, Chem. Phys. Letts. 285, 163 (1998).
7. "Quantum Wave Packet Dynamics of van der Waals Fragmentation", Meishan Zhao, Soonmin Jang and Stuart A. Rice, Internet Journal of Chemistry 1, 1999v2/1/, (1999).
8. "Quantum molecular dynamics simulations of low temperature high energy density matter: solid p-H<sub>2</sub>/Li and p-H<sub>2</sub>/B", Soonmin Jang, Seogjoo Jang, and Gregory. A. Voth, J. Phys. Chem. A, 103, 9512(1999).
9. "Quantum Dynamical Simulation of the Energy Relaxation Rate of the CN<sup>-</sup> Ion in Water", Soonmin Jang, Youngshang Pak, Gregory A. Voth, J. Phys. Chem. A, 103, 10289(1999), (Kent Wilson Festschrift).
10. "Centroid Molecular Dynamics: A Quantum Dynamics Method Suitable for the Parallel Computer", Marc Pavese, Soonmin Jang, and Gregory A. Voth, Parallel computing, 26, 1025 (2000).
11. "Application of a higher order composite factorization schemes in imaginary time path integral simulation", Seogjoo Jang, Soonmin Jang, and Gregory A. Voth, J. Chem. Phys. 115, 7832(2001).
12. "Quantum molecular dynamics and spectral simulation of a boron impurity in

- solid para-hydrogen", Jennifer Krumrine, Soonmin Jang, Millard H. Alexander, and Gregory A. Voth, *J. Chem. Phys.* 113, 9079(2000).
13. "Multicanonical ensemble with Nose-Hoover chain dynamics simulation", Soonmin Jang, Youngshang Pak, and Seokmin Shin, *J. Chem. Phys.* 116, 4782(2002).
  14. "Prediction of helical peptide folding in an implicit water by a new molecular dynamics scheme with generalized effective potential", Youngshang Pak, Soonmin Jang, and Seokmin Shin, *J. Chem. Phys.* 116, 6831(2002).
  15. "Molecular Dynamics Study of Peptides in Implicit Water: Ab Initio Folding of  $\beta$ -Hairpin,  $\beta\beta$ -Sheet, and  $\beta\beta\alpha$ -motif", Soonmin Jang, Seokmin Shin, and Youngshang Pak, *JACS Comm.* 124, 4976(2002)
  16. "Replica-Exchange Method Using the Generalized Effective Potential", Soonmin. Jang, Seokmin. Shin, and Youngshang. Pak, *Phy. Rev. Lett.* 91, 058305(2003)
  17. "Folding dynamics of beta-hairpins: molecular dynamics simulations", Jinhyuk Lee, Soonmin Jang, Youngshang, and Seokmin Shin, *Bull. Korean. Chem. Soc.* 24, 785(2003).
  18. "Ab initio folding of helix bundle proteins using Molecular Dynamics simulations", Soonmin Jang, Eunae Kim, Seokmin Shin, and Youngshang Pak, *J. Am. Chem. Soc.* 125, 14841(2003).
  19. "Structure of 4-biphenylthiolate on Au Nanoparticle Surfaces Studied by UV-Vis Absorption Spectroscopy, Transmission Electron Microscopy and Surface-enhanced Raman Scattering", Soonmin Jang, Sunil Kim, Seokmin Shin, Sang Woo Joo, *Surface and Interface Analysis*, 36, 43 (2004).
  20. "Adsorption of 4-Biphenylmethanethiolate on Different-Sized Gold Nanoparticle Surfaces", Soonmin Jang, Jingsung Park, Seokmin Shin, Changjung Yoon, Byoung Koo Choi, Myoung-seon Gong, and Sang-Woo Joo, *Langmuir* 20, 1922 (2004)
  21. "Quantum Phase Transition of Water Clusters: Molecular Dynamics Simulations with a Model Potential", Seokmin Shin, Wonjun Son, and Soonmin Jang, *J. Mol. Str. – Theochem*, 673, 109 (2004).
  22. "Asymmetric nucleophilic substitution of  $\alpha$ -bromo amides via dynamic kinetic resolution for the preparation of dipeptide analogues", Jiyoung Nam, Ji-yeon Chang, Eun-kyoung Shin, Hyun Jung Kim, Yangmee Kim, Soonmin Jang and Yong Sun Park, *Tetrahedron*, 60, 6311 (2004).
  23. "Misfolded free energy surface of a peptide with  $\alpha$ - $\beta$ ,  $\beta$ - $\beta$  motif", Youngshang Pak, Eunae Kim, and Soonmin Jang, *J. Chem. Phys.* 121, 9184 (2004).
  24. "Amyloid A $\beta$ -Peptide Oligomerization in Silico: Dimer and Trimer", Soonmin Jang, Seokmin Shin, *J. Phys. Chem. B*, 110, 1995 (2006).
  25. "Free Energy Surfaces of Mini-proteins with  $\beta\beta\alpha$  Motif: Replica Exchange Molecular Dynamics Simulation with an Implicit Solvation Model", Soonmin Jang, Eunae Kim, Youngshang Pak, *PROTEINS: Str. Func. and Bioinfor.*, 62, 663 (2006)
  26. "Theoretical investigation of the photoinitiated folding of HP-36", Soonmin Jang, Narasima Sereerama, Vivian H.-C. Liao, S. H-F Lu, Feng-Yin Li, Seokmin Shin, R. W. Woody, and S. H. Lin, *Protein Sci.*, 15, 2290 (2006).

27. "Direct Folding Simulation of  $\alpha$ -helices and  $\beta$ -hairpins based on a Single All-atom Force Field with an Implicit Solvation Model", Soonmin Jang, Eunae Kim, Youngshang Pak, *PROTEINS: Str. Func. and Bioinfor.*, 66, 53 (2007).
28. "Folding simulations with novel conformational search method", Won-Joon Son, Soonmin Jang, Youngshang Pak, and Seokmin Shin, *J. Chem. Phys.* 126, 104906 (2007).
29. "Abnormal adsorption behavior of dimethyl disulfide on gold surfaces", Jaegeun Noh, Soonmin Jang, Donghyung Lee, Seokmin Shin, Younh Joon Ko, Eisuke Ito, Sang-Woo Joo, *Current Applied Physics*, 7, 605 (2007).
30. "Consistent free energy landscapes and thermodynamic properties of small proteins based on a single all-atom force field employing an implicit solvation", Eunae Kim, Soonmin Jang, Youngshang Pak, *J. Chem. Phys.* 127, 145104 (2007).
31. "Synthesis and conformational study of Ser and Cys derivatives of N-Hydroxy Diketopiperazine", S-W. You, W. Park, Hyoung-Tae Lee, Jeonghoon Ueom, Soonmin Jang, Kyunghye Lee, and Dongyeoul Lim, *Bull. Kor. Chem. Soc.* 28, 2414 (2007).
32. "All atom level direct folding simulation of  $\beta$ -amini-protein", Soonmin Jang, Eunae Kim, and Youngshang pak, *J. Chem. Phys.* 128, 105102 (2008).
33. "Conformational characteristics of unfolded or misfolded peptides", Jaesung Yoon, Joonho Park, Soonmin Jang, Kyunghye Lee, and Seokmin Shin, *J. Biomolecular Structure and Dynamics*, 25, 505 (2008).
34. "Computational study of structural diversity of amyloid beta peptide (A $\beta$ 10-35) oligomers", Soonmin Jang and Seokmin Shin, *J. Phys. Chem. B.* 112, 3479 (2008).
35. "Direct folding studies of various  $\alpha$ - and  $\beta$ - strands using replica exchange molecular dynamics simulation", Eunae Kim,<sup>1</sup> Soonmin Jang,<sup>2</sup> and Youngshang Pak<sup>1</sup>, *J. Chem. Phys.* 128, 175104 (2008).
36. "Free energy landscapes of a highly structured  $\beta$ -hairpin peptide and its single mutant", Eunae Kim, Changwon Yang, Soonmin Jang, and Youngshang Pak, *J. Chem. Phys.* 129, 165104 (2008).
37. "Interfacial interactions and dispersion relations in carbon–aluminium nanocomposite systems", Woong Lee, Soonmin Jang, Min Jun Kim, and Jae-Min Myoung, *Nanotechnology*, 19, 285701 (2008)
38. "A simple method of estimating sampling consistency based on free energy map distance", Won-Joon Son, Soonmin Jang, Seokmin Shin, *J. Mol. Graph. & Modell.*, 27, 321 (2008)
39. "Site Specificity of the  $\alpha$  C-H Bond Dissociation Energy for a Naturally Occurring  $\beta$ -Hairpin Peptide—An Ab Initio Study", Wan-Chun Cheng, Soonmin Jang, Chen-Changwu, Ren-Jie Lin, Hsiu-Feng Lu, Feng-Yin Li, *J. Comp. Chem.* 30, 407 (2009).
40. "Structural Properties of Fibril-forming Segments of  $\alpha$ -Synuclein, Jeseong Yoon, Joonho Park, Soonmin Jang, Kyunghye Lee, and Seokmin Shin, *Bull. Kor. Chem. Soc.* 30, 654 (2009)

41. "Dimerization of Fibril-forming Segments of  $\alpha$ -Synuclein", Jeseong Yoon, Soonmin Jang, Kyunghee Lee, and Seokmin Shin, *Bull. Kor. Chem. Soc.* 30, 1845 (2009)
42. "Computational Study of Human Calcitonin (hCT) Oligomer", Youngshang Pak, Jungho Shin, and Soonmin Jang, *Bull. Kor. Chem. Soc.* 30, 3006 (2009).
43. "Comparison of ionization behaviors of ring and linear carbohydrates in MALDI-TOFMS", Sung-Seen Choi, Hye Min Lee, Soonmin Jang, Jungho Shin, *Int. J. of Mass Spectrometry*, 279 53 (2009)
44. "All-atom *ab initio* native structure prediction of a mixed fold (1FME): A comparison of structural and folding characteristics of various  $\beta\alpha\alpha$  miniproteins", Eunae Kim, Soonmin Jang, Youngshang Pak, *J. Comp. Phys.* 131, 195102 (2009)
45. "Energy Landscapes Associated with the Self-Aggregation of an Alanine-Based Oligopeptide (AAKA)<sub>4</sub>" Soonmin Jang, Jian-Min Yuan, Jungho Shin, Thomas J. Measey, Reinhard Schweitzer-Stenner, and Feng-Yin Li, *J. Phys. Chem. B*, 113, 6054 (2009)
46. "Crystal Structure of the TNF $\alpha$ -Inducing Protein (Tip $\alpha$ ) from *Helicobacter pylori*: Insights into Its DNA-Binding Activity", Jun Young Jang, Hye-Jin Yoon, Ji Young Yoon, Hyoun Sook Kim, Sang Jae Lee, Kyoung Hoon Kim, Do Jin Kim, Soonmin Jang, Byeong-Gu Han, Byung Il Lee, Se Won Suh, *J. Mol. Biol.* 392, 191 (2009)
47. "Geometric Effects on Conductance in Single Molecule Electron Transport Junctions" Shang-Chieh Hsieh, Fur-Der Mai, Soonmin Jang, Hong-Yi Tang, and Feng-Yin Li, *J. Chinese Chem. Soc.*, 56, 1198 (2009)
48. "On the Structural Stability of a Short Three Stranded  $\beta$ -sheet Peptide (Betanova): Replica Exchange Molecular Dynamics Simulation Study", Soonmin Jang, Eunae Kim, and Youngshang Pak, *Bull. Korean Chem. Soc.* 31, 2386 (2010).
49. "Free Energy Landscape of the FBP28 WW Domain by All-Atom Direct Folding Simulation" Eunae Kim, Soonmin Jang, Manho Lim, and Youngshang Pak, *J. Phys. Chem. B*, 114, 7686 (2010)
50. "Variation of reaction dynamics for OH hydrogen abstraction from glycine between *ab initio* levels of theory", Ren-Jie Lin & Chen-Chang Wu & Soonmin Jang, Feng-Yin Li *J. Mol. Model.* 16, 175 (2010).
51. "Docking study of the precursor peptide of mastoparan onto its putative processing enzyme, dipeptidyl peptidase IV: a revisit to molecular ticketing", Soonmin Jang, Tse-Yu Chung, Jungho Shin, Kai-Lun Lin, Jason T. C. Tzen, Feng-Yin Li, *J. Comput. Aided Mol Des.* 24, 213 (2010).
52. "A Naked Eye Detection of Fluoride with Urea Receptors Which have both an Azo Group and a Nitrophenyl Group as a Signaling Group", Nhat Tuan Dang, Jin Joo Park, Soonmin Jang, Jongmin Kang, *Bull. Kor. Chem. Soc.* 31, 1204 (2010).
53. "Carboxylate selective anion receptor based on two anthracenes with malonamide spacer", Sung Kyu Lee, Hyunsik Kim, Soonmin Jang, Jongmin Kang, *Tetrahedron Letters*, 52, 1977 (2011).
54. "Formation of metal complex ions from amino acid in the presence of Li<sup>+</sup>, Na<sup>+</sup> and K<sup>+</sup> by electrospray ionization: metal replacement of hydrogen in the

- ligands”, Soonmin Jang, Min Ju Song, Hyunsik Kim and Sung-Seen Choi, *J. Mass. Spectrom.*, 46, 496 (2011)
55. “Phase Transition of Confined Gold Nanoparticles: Replica Exchange Molecular Dynamics Study”, Hyunsik Kim, F-Y Li, Soonmin Jang, *Bull. Kor. Chem. Soc.* 33, 929(2012).