Hongsuk Kang

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EDUCATION

UNIVERSITY OF MARYLAND **College Park, MD**
Ph.D of Chemical Physics 8/2014
Dissertation title "Jamming effects in glasses and biopolymers"
Advisor: **Prof. Devarajan Thirumalai**

SEOUL NATIONAL UNIVERSITY **Seoul, Korea**
Bachelor of Science, *cum laude,* Double major in Physics and Computer Science 2/2001

EXPERIENCE

IBM THOMAS J. WATSON RESEARCH CENTER **Yorktown Heights, NY**
Postdoctoral Researcher – Computational Biology Center: Supervisor-Ruhong Zhou 6/2015-6/2018

- Conduct research projects initiated by non-profit organization about relating protein structures to incurable neurodegenerative disease development using all-atom molecular dynamics (MD) simulation with enhanced sampling method on IBM BlueGene/Q
- Design and perform self-motivated scientific research projects regarding prevention of protein aggregation and disease progression in human eyes using all-atom MD simulations on GPU clusters

UNIVERSITY OF MARYLAND **College Park, MD**
Research Assistant – Professor Devarajan Thirumalai 5/2009-6/2015

- Lead research related to thermodynamic properties of DNA and RNA under macromolecular crowding environment using coarse grained model
- Perform large scale molecular dynamics simulation using Brownian and Newtonian dynamics scheme and analyze data to estimate thermodynamic properties of colloidal suspensions

UNIVERSITY OF MARYLAND **College Park, MD**
Teaching Assistant – Physical Chemistry Lab 1/2014-5/2014
8/2008-5/2009

- Instruct and supervise undergraduate students during the lab sessions and grade the experiment reports

KOREA RESEARCH INSTITUTE OF BIOSCIENCE AND BIOTECHNOLOGY
Daejon, Korea
Researcher – Division of Biomedical Genomics Research Center 3/2006-2/2007
Researcher – National Genome Information Center 3/2005-2/2006

- Develop potential energy function for hydrogen bond between side chain analogues of amino acids using Density Functional Theory calculations
- Improve solvation free energy function in AUTODOCK by introducing new atom types and optimizing parameters with genetic algorithm

IUTECH, *Inc* **Busan, Korea**
Developer – Software team (alternative to mandatory military service) 5/2001-8/2004

- Design, develop and test client program for Windows and relay server product supplied with network

digital video recorder

SAMSUNG ADVANCED INSTITUTE OF TECHNOLOGY **Gyeonggi, Korea**
Intern – Computational Science and Engineering Lab 7/2000-8/2000, 1/2001-2/2001

- Produce a visualization tool for the simulation data of amorphous LCD recrystallization process
- Create graphic user interface for job submissions to the cluster

SKILLS

Computer

- Highly proficient (over 15 years of experience) in programming languages such as C/C++, Java, SQL, Perl, Python and shell script (bash).
- Proficient in parallelization using MPI and CUDA code

Scientific tools: Proficient in Mathematica, NAMD, GROMACS, LAMMPS, Gaussian and GAMESS

PUBLICATIONS

Choi, H., **Kang, H.**, Chung, K.C., Park, H., "Development and application of a comprehensive machine learning program for predicting molecular biochemical and pharmacological properties" Phys. Chem. Chem. Phys. 21 (9), 5189 (2019)

Kang, H., Luan, B., Zhou, R., "Glassy Dynamics in Mutant Huntingtin Proteins", J. Chem. Phys., 149, 072333 (2018)

Kang, H., Yang, Z., Zhou, R., "Lanosterol disrupts aggregation of human γD-crystallin by binding to the hydrophobic dimerization interface", J. Am. Chem. Soc., 140(27), 8479 (2018)

Kang, H., Vazquez, F. X., Zhang, Z., Das, P., Toledo-Sherman, L., Luan, B., Levitt, M., Zhou, R., "Emerging β-sheet Rich Conformations in Super-compact Huntingtin Exon-1 Mutant Structures", J. Am. Chem. Soc., 139(26), 8820 (2017)

Zhang, Z., **Kang, H.**, Vazquez, F. X., Toledo-Sherman, L., Luan, B., Zhou, R., "Molecular Mechanism of Stabilizing the Helical Structure of Huntingtin N17 in a Micellar Environment", J. Phys. Chem. B, 121(18), 4713 (2017)

Feng, M., **Kang, H.**, Yang, Z., Luan, B., Zhou, R. "Potential disruption of protein-protein interactions by graphene oxide" J. Chem. Phys., 144, 225102 (2016)

Meng, XY., Li, B., Liu S., **Kang, H.**, Zhao, L., Zhou, R. "EGCG in Green Tea Induces Aggregation of HMGB1 Protein through Large Conformational Changes with Polarized Charge Redistribution" Sci. Rep., 6 (2016)

Kang, H., Yoon, YG., Thirumalai, D. and Hyeon, C., "Confinement-induced glassy dynamics in a model for chromosome organization" Phys. Rev. Lett., 115, 198102 (2015)

Choi, H., **Kang, H**., and Park, HS "Scaled Particle Theory and Free-Energy Perturbation Method" J. Chem. Theo. Comp., 11, 4933 (2015) [co-first author]

Kang, H., Toan MN., Hyeon, C., and Thirumalai, D, "Unexpected Swelling of Stiff DNA in a Polydisperse Crowded Environment" J. Am. Chem. Soc., 137, 10970 (2015)

Kang, H., Pincus, PA., Hyeon, C., and Thirumalai, D, “Effects of macromolecular crowding on the collapse of biopolymers” Phys. Rev. Lett., 114, 068303 (2015)

Kang, H., Kirkpatrick, TR, and Thirumalai, D., “Manifestation of Random First Order Transition theory in Wigner glasses” Phys. Rev. E, 88, 042308 (2013)

Choi, H., **Kang, H**., and Park, HS “Extended solvent-contact model for protein solvation: Test cases for dipeptides” J. Mol. Graphics Modell., 42, 50 (2013) [co-first author]

Choi, H., **Kang, H**., and Park, HS “New solvation free energy function comprising intermolecular solvation and intramolecular self-solvation terms” J. Chem. Inf., 5, 8 (2013)

Choi, H., **Kang, H**., and Park, HS “MetLigDB: a web-based database for the identification of chemical groups to design metalloprotein inhibitors” J. Appl. Cryst., 31, 878 (2011) [co-first author]

Choi, H., **Kang, H**., and Park, HS “New Angle-Dependent Potential Energy Function for Backbone-Backbone Hydrogen Bond in Protein-Protein Interactions” J. Compu. Chem., 31, 897 (2010) [co-first author]

Choi, H., **Kang, H**., and Park, HS “Extended Morse Function Model for Angle-Dependent Hydrogen Bond in Protein-Protein Interactions” J. Phys. Chem. B., 114, 2980 (2010) [co-first author]

Kang, H., Choi, H. and Park, HS “Prediction of molecular solvation free energy based on the optimization of atomic solvation parameters with genetic algorithm” J. Chem. Inf. Mod., 47, 509 (2007) [co-first author]