

# 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

### INSTITUTE FOR BIOSCIENCE AND BIOTECH RESEARCH, UNIVERSITY OF MARYLAND

Rockville, MD

*Postdoctoral Associate*

### NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

Gaithersburg, MD

*Guest Researcher*

- Develop a numerical model for and computationally research about properties and aggregation profiles of Monoclonal Antibody (mAB) at high concentration.

### 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

Daejeon, 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  $\gamma$ D-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  $\beta$ -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]