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A. ACDEMIC QUALIFICATIONS

- University at Buffalo, The State University of New York (SUNY Buffalo)
Ph.D. in Chemical and Biological Engineering – Presidential Fellow, 06/2005
Thesis: *Studies of Point Defects in Strained Solids by Molecular Simulation*
- University at Buffalo, The State University of New York (SUNY Buffalo)
B.S. in Chemical Engineering - Summa Cum Laude, HoneyWell Inc. Fellow, 06/1999

MEMBERSHIPS

- Member of Korean Institute of Chemical Engineers (KIChE), 05/2012 – present
- Member of American Chemical Society (ACS), 09/2011 – present
- Member of American Institute of Chemical Engineering (AIChE), 11/2003 – present
- Member of American Nano Society (ANS), 2011 – present
- Member of Golden Key honor society, 08/1998 – present
- Member of Tau Beta Pi engineering honor society, 08/1998 – present
- Editorial Board Member of Journal of Periodontal & Implant Science, 2009 – present
- Editorial Board Member of Dataset Papers in Atomic and Molecular Physics, 2012 – present

WORK EXPERIENCES

- Associate Professor, 09/2014-current, School of Energy and Chemical Engineering, UNIST
- Chair of Department of Chemical Engineering (ACE), 01/2014 – current , School of Energy and Chemical Engineering, UNIST
- Coordinator of Chemical Engineering Track (ACE), 04/2012 – 12/2013 , School of Nano-Bioscience and Chemical Engineering, UNIST
- Assistant Professor, 02/2012-08/2014, School of Nano-Bioscience and Chemical Engineering, UNIST (started from Feb. 3, 2012)
- Assistant Professor, School of Chemical and Biomedical Engineering 06/2005 – 12/2011 at Nanyang Technological University (NTU), Singapore
- Research and Teaching Assistants, University at Buffalo, SUNY, 01/2000 – 06/2005
- Research Assistant in Buffalo R&D department, HoneyWell Inc., Buffalo, NY, 08/98 – 12/98
- Undergraduate Research Assistant, University at Buffalo, SUNY, 09/98 – 12/98

B. RESEARCH

- **Research Background**

Molecular Modeling and Simulation, Molecular Physics, Thermodynamics, Chemical Engineering, Statistical Mechanics

- **Research Interest**

Energy, Materials, Environment, Health, and Fundamental Studies on Phase Equilibria

1. Bora Seo, Gwan Yeong Jung, Young Jin Sa, Hu Young Jeong, Jae Yeong Cheon, Jeong Hyeon Lee, Ho Young Kim, Jin Chul Kim, Hyeon Suk Shin, Sang Kyu Kwak*, and Sang Hoon Joo*, "Monolayer-Precision Synthesis of Molybdenum Sulfide Nanoparticles and Their Nanoscale Size Effects in the Hydrogen Evolution Reaction", *ACS Nano*, 2015 (DOI:10.1021/acsnano.5b00786)
2. Sa Hoon Min, Sang Kyu Kwak*, and Byeong-Su Kim*, "Atomistic simulation for coil-to-globule transition of poly(2-dimethylaminoethyl methacrylate)", *Soft Matter*, 11, 2423-2433, 2015
3. Hye Hyun Kim, Minhak Oh, Dongwook Kim, Jeongin Park, Junmo Seong, Sang Kyu Kwak, and Myoung Soo Lah*, "Single crystalline hollow metal-organic frameworks: a metal-organic polyhedron single crystal as a sacrificial template", *Chemical Communications*, 51, 3678-3681, 2015
4. Moo Yeol Lee, Hyeong Jun Kim, Gwan Yeong Jung, A-Reum Han, Sang Kyu Kwak, Bumjoon J. Kim*, and Joon Hak Oh* "Highly Sensitive and Selective Liquid-Phase Sensors Based on a Solvent-Resistant Organic Transistor Platform", *Advanced Materials*, 27(9), 1540-1546, 2015 Inside Front Cover.
5. Se Hun Joo, Ji Hye Seong, Jin Sol Han, Ju An Yang, and Sang Kyu Kwak* "Study of Quaternary System of Salicylic Acid, Water, Ozone, and PAL by Molecular Dynamics ", *Fluid Phase Equilibria*, 388, 43, 2015.
6. Ji-Hoon Park, Dae-Hyun Cho, Youngkwon Moon, Ha-Chul Shin, Sung-Joon Ahn, Sang Kyu Kwak, Hyeon-Jin Shin, Changgu Lee, and Joung Real Ahn, "Designed three-dimensional freestanding single-crystal carbon architectures", *ACS Nano*, 2014 (DOI: 10.1021/nn504956h)
7. Boseok Kang, Moonjeong Jang, Yoonyoung Chung, Haena Kim, Sang Kyu Kwak, Joon Hak Oh*, and Kilwon Cho*, "Enhancing 2-D Growth of Organic Semiconductor Thin Film with Macroporous Structures via Small Molecule Heterointerface", *Nature Communications*, 5:4752, 2014
8. Byeong Soo Shin, Eun Sung Kim, Sang Kyu Kwak, Jong Sung Limd, Ki-Sub Kim* and Jeong Won Kang*, "Thermodynamic Inhibition Effects of Ionic Liquids on the Formation of Condensed Carbon Dioxide Hydrate", *Fluid Phase Equilibria*, 382, 270-278, 2014.
9. Gwan Yeong Jung, Woo Chul Jeon, Eun Hae Shin, and Sang Kyu Kwak*, "Application of Multiscale Molecular Modeling and Simulation Methods", *News & Information for Chemical Engineers*, 32(6), 775-779, 2014. (Magazine)
10. Piyaat Weerachanchai, Sang Kyu Kwak, and Jong-Min Lee, "Effects of Solubility Properties of Solvents and Biomass on Biomass Pretreatment", *Bioresource Technology*, 170C, 160-166, 2014.
11. Su Hwan Kim, Tae Kyung Lee, Tae-Il Kim*, and Sang Kyu Kwak*, "Effect of Ga and As Vacancies on Electronic Properties of Ga_{0.9375}Al_{0.0625}As", *Molecular Physics*, 112(22), 2970-2978, 2014.
12. Ga Eun Son, Nyambayar Sugartseren, Won Byong Yoon, and Sang Kyu Kwak*, "Phase Behavior of Ternary Mixture of Water-Vanillin-Ethanol in Vanillin Extraction via Dissipative Particle Dynamics ", *Journal of Chemical & Engineering Data*, 59(10), 3036-3040, 2014.
13. Huan Cong Huang, Pei-Chen Su, Sang Kyu Kwak, Rojana Pornprasertsuk, and Yong-Jin Yoon, "Molecular Dynamics Simulation of Oxygen Ion Diffusion in Yttria Stabilized Zirconia Single Crystals and Bicrystals", *Fuel Cells*, 14(4), 574-580, 2014.
14. Tae Kyung Lee and Sang Kyu Kwak*, "Effects of LSPR of Gold Nanospheres by Surface Vacancies and Protruding Tips", *Journal of Physical Chemistry C*, 118(11), 5881, 2014.

15. Tae Kyung Kim, Kyung Joo Lee, Junhan Yuh, Sang Kyu Kwak, and Hoi Ri Moon, "Multi-core MgO NPs@C core-shell nanospheres for selective CO₂ capture at mild condition", **New Journal of Chemistry**, 38, 1606-1610, 2014.
16. Chao Liu, Sang Kyu Kwak*, and Ansumali Santosh*, "Direct Simulation Monte Carlo for Dense Hard Spheres", **International Journal of Modern Physics C**, 25(1), 1340023, 2014.
17. Kyungil Kong, Biplab K. Deka, Sang Kyu Kwak, Aeri Oh, Heejune KIM, Young-Bin Park*, and Hyung Wook Park*, "Processing and Mechanical Characterization of ZnO/Polyester Woven Carbon-Fiber Composites with Different ZnO Concentrations", **Composites Part A: Applied Science and Manufacturing**, 55, 152-160, 2013.
18. Huan Cong Huang, Yong-Jin Yoon, and Sang Kyu Kwak*, "On the Freezing and Structure of Hard-Spheres under Spherical Confinement", **Molecular Physics**, 111(21), 3283-3288, 2013.
19. Wen Wen Chen, Yong-Jin Yoon, Su Jan Susanna Leong*, and Sang Kyu Kwak*, "Study of Dimerization of HBD and Its Interactions with POPG Membrane", **Molecular Simulation**, 39(11), 849-859, 2013.
20. Xue Tong, Xin Wang, Sang Kyu Kwak, and Jong-Min Lee*, "Synthesis and Application of Mesoporous Polyaniline (PANI)-Se_{0.5}Te_{0.5} Dual-Layer Electrodes by Lyotropic Liquid Crystalline Templates as Direct Cast", **Industrial & Engineering Chemistry Research**, 52(14), 5072-5078, 2013.
21. Xiang Li, Rathi Saravanan, Sang Kyu Kwak*, and Susanna Su Jan Leong*, "Biomolecular engineering of a human beta defensin model for increased salt resistance", **Chemical Engineering Science**, 95, 128-137, 2013.
22. Sang Kyu Kwak* and Ken-Tye Yong, "Effects of Low-Order Surface Vacancy on Extinction Spectra of Localized Surface Plasmon Resonance", **Journal of Computational and Theoretical Nanoscience**, 9(10), 1642-1646, 2012.
23. Tong Xue, L. S. Loo, Xin Wang, Sang Kyu Kwak, and Jong-Min Lee*, "Electrodeposition of Mesoporous Bilayers of Polyaniline Supported Cu₂O Semiconductor Films from Lyotropic Liquid Crystalline Phase", **Chemical Engineering Science**, 80, 452-459, 2012.
24. Ken-Tye Yong, Yucheng Wanga, Indrajit Roy, Hu Rui, Mark T. Swihart, Wing-Cheung Lawd, Sang Kyu Kwak, Ling Ye, Jianwei Liu, Supriya D. Mahajan, and Jessica L. Reynolds, "Preparation of Quantum Dot/Drug Nanoparticle Formulations for Traceable Targeted Delivery and Therapy", **Theranostics**, 2(7), 681-694, 2012.
25. Wen Wen Chen, Derrick Tay Kok Sing, Susanna Su Jan Leong and Sang Kyu Kwak*, "Three Dimensional Structure of Human Beta-Defensin 28 via Homology Modeling and Molecular Dynamics", **Molecular Simulation**, 38(2), 90-101, 2012.
26. Sang Kyu Kwak*, Taezoon Park, Yong-Jin Yoon, and Jong-Min Lee, "Estimation of the Free Energy of Hard-Sphere Crystal via Free-Volume Approach", **Molecular Simulation**, 38(1), 16-22, 2012.
27. Jong Dae Baek, Yong-Jin Yoon, Mohammad Hossein Abedin Nasab, Beihei Han, and Sang Kyu Kwak, "Estimation of Optimal Insertion Angle in a Mammalian Outer Hair Cell Stereocilium", **Journal of Biomechanics**, 45, 1823-1827, 2012.
28. Huan Cong Huang, Jayant K. Singh, Jong-Min Lee, and Sang Kyu Kwak*, "Confining Effect of Carbon-Nanotube Configuration on Phase Behavior of Hard-Sphere Fluid", **Fluid Phase Equilibria**, 318, 19-24, 2012.
29. Kyung-Don Nam, Sang Kyu Kwak, and Jong-Min Lee, "Synthesis of ZnO nanorods by the thermal reduction process of the mixture of ZnO and Al powder", **Crystal Research and Technology**, 46, 1323-1328, 2011.

30. Liu Chao, Pei-Chen Su, and Sang Kyu Kwak*, “Generalized Equilibrium Concentration of Polyvacancy: Case study for Trivacancy in Hard-Sphere Crystals”, **Molecular Physics**, 109, 2461-2470, 2011.
31. Huan Cong Huang, Wen Wen Chen, Jayant K. Singh, and Sang Kyu Kwak*, “Direct Determination of Fluid-Solid Coexistence of Square-Well Fluids Confined in Narrow Cylindrical Hard Pore”, **Journal of Chemical Physics**, 132(22), 224504, 2010.
32. Wen Wen Chen, Huan Cong Huang and Sang Kyu Kwak*, “Evaluation of Bridge Function for Hard Sphere Fluid Confined in a Narrow Slit-pore via TMMC Mayer-Sampling”, **Molecular Physics**, 108(11), 1531-1537, 2010.
33. Liang Yu Yan, Weifeng Li, Xiao Feng Fan, Wei Li, Yuan Chen, Jer-Lai Kuo, Lain-Jong Li, Sang Kyu Kwak, Yuguang Mu, M.B. Chan-Park, “Enrichment of (8,4) single-walled carbon nanotubes through co-extraction with heparin”, **Small**, 6(1), 110-118, 2010.
34. Wahyu Perdana Yudistiawan, Sang Kyu Kwak, D.V. Patil, and Santosh Ansumali*, “Higher-Order Galilean-invariant lattice Boltzmann Model for Microflows: Single Component Gas”, **Physical Review E**, 82, 046702, 2010.
35. Sudhir K. Singh, Jayant K. Singh*, Sang Kyu Kwak, and Goutam Deo, “Phase Transition and Crossover Behavior of Colloidal Fluids under Confinement”, **Chemical Physics Letters**, 494, 182-187, 2010.
36. Wen Wen Chen and Sang Kyu Kwak*, “Calculation of bridge function coefficients via modified Mayer-sampling”, **Molecular Physics**, 107, 2213-2220, 2009.
37. Ashim K. Saha, Satya P. Singh, Jayant K. Singh*, and Sang Kyu Kwak, “Quasi-2D and prewetting transitions of square-well fluids on a square-well substrate, **Molecular Physics**, 107, 2189-2200, 2009
38. Subimal Jana, Jayant K. Singh*, and Sang Kyu Kwak, “Vapor-liquid critical and interfacial properties of square-well fluids in slit pores”, **Journal of Chemical Physics**, 130, 214707, 2009
39. Huan Cong Huang, Sang Kyu Kwak*, and Jayant K. Singh, “Characterization of Fluid-Solid Phase Transition of Hard Sphere Fluids in Cylindrical Pore via Molecular Dynamics Simulation”, **Journal of Chemical Physics**, 130, 164511, 2009.
40. Panji Gazali, Sang Kyu Kwak*, and Jayant K. Singh, “Interface mixing behaviour of Lennard-Jones FCC (100) thin film”, **Molecular Physics**, 106, 2417-2423, 2008.
41. Sang Kyu Kwak*, Yenni Cahyana, and Jayant K. Singh, “Characterization of mono- and divacancy in fcc and hcp hard-sphere crystals”, **Journal of Chemical Physics**, 128, 13514, 2008.
42. Jayant K. Singh*, Gautam Sarma, and Sang Kyu Kwak, “Thin-thick surface phase-coexistence and boundary tension of the square-well fluid”, **Journal of Chemical Physics**, 128, 044708, 2008.
43. Sang Kyu Kwak*, Jayant K. Singh*, and Adhikari Jhumpa, “Molecular simulation study of vapor-liquid equilibrium of Morse fluids”, **Chemical Product and Process Modeling**, 2(3), 2007.
44. Jayant K. Singh* and Sang Kyu Kwak*, “Surface tension and vapor-liquid phase coexistence of confined square-well fluid”, **Journal of Chemical Physics**, 126(2), 024702, 2007.
45. Jayant K. Singh*, Adhikari Jhumpa and Sang Kyu Kwak, “Interfacial properties of Morse fluids”, **Molecular Physics**, 105(17-18), 2327, 2007.
46. Jayant K. Singh*, Adhikari Jhumpa and Sang Kyu Kwak, “Interfacial properties of Morse fluids”, **Molecular Physics**, 10, 5(8), 981-987, 2007.
47. Jayant K. Singh*, Adhikari Jhumpa*, and Sang Kyu Kwak*, “Vapor-liquid phase coexistence curves for Morse fluids”, **Fluid Phase Equilibria**, 248(1), 1-6, 2006.

48. Sang Kyu Kwak and David. A. Kofke*, “Effect of monovacancies on the relative stability of fcc and hcp hard-sphere crystals”, [Journal of Chemical Physics](#), 122, 176101, 2005.
49. Sang Kyu Kwak and David. A. Kofke*, “Evaluation of bridge-function diagrams via Mayer-sampling Monte Carlo simulation”, [Journal of Chemical Physics](#), 122, 104508, 2005.
50. Sang Kyu Kwak and David. A. Kofke*, “Elastic constants and the effect of strain on monovacancy concentration in FCC hard-sphere crystals”, [Physical Review B](#), 70, 214113, 2004.

Published Book Chapter

1. Sang Kyu Kwak* and Jayant K. Singh*, “Understanding the freezing and melting behavior under confinement”, CRC Press, Taylor and Francis Group, Edited by Beena Rai, 2012. (Book Title: *Molecular Modeling for the Design of Novel Performance Chemicals and Materials*)