

Tonglei Li

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CONTACT INFORMATION:

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EDUCATION

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- 1999 Ph. D. in Pharmaceutics  
Purdue University, West Lafayette, IN. Advisor: (b) (6)  
Thesis: *Fractal Analysis of Surface Roughness and Study of Etching Mechanism of Acetaminophen Single Crystals*
- 1997 M.S. in Computer Science  
Purdue University, West Lafayette, IN.
- 1991 M.S. in Computational Chemistry  
Nankai University, Tianjin, China  
Advisor: (b) (6)
- 1988 B.S. in Chemistry  
Nankai University, Tianjin, China

PROFESSIONAL EXPERIENCES

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- 2014- Associate Dean for Graduate Programs, College of Pharmacy
- 2012- Professor and Allen Chao Chair in Industrial & Physical Pharmacy
- 2012- Faculty Member, The Engineering Research Center for Structure Organic Particulate System, Purdue University
- 2013- Faculty Member, Computational Science & Engineering, Purdue University
- 2013- Faculty Member, Biotechnology Training Group, Interdisciplinary Life Science Program (PULSE), Purdue University
- 2007- Associate Professor of Pharmaceutics, University of Kentucky  
2012
- 2005- Markey Cancer Center, University of Kentucky  
2012
- 2002- Assistant Professor of Pharmaceutics, University of Kentucky  
2007
- 1999- Visiting Assistant Professor of Pharmaceutics,  
2002 Purdue University  
Mentor: (b) (6)

1993- Graduate Research Assistant, Purdue University  
1999  
1991- Research Scientist, Nankai University, China  
1993  
1988- Graduate Research Assistant, Nankai University, China  
1991

#### HONORS AND AWARDS

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2013 AAPS Fellow  
2012 Alan Chao Chair  
2007 Robert A. Blouin Excellence in Graduate Education Award  
(University of Kentucky, College of Pharmacy)  
2006 DOD Breast Cancer Idea Award  
2005 NSF CAREER Award  
2004 AACP New Investigator Award  
2004 DOD Breast Cancer Concept Award  
2003 PhRMA Research Starter Award  
2002 AAPS New Investigator Award  
1998 Pharmacia-Upjohn Walter F. Enz Award

#### PROFESSIONAL ACTIVITIES

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Editor: Pharmaceutical Research (2015 - )

Editorial Board:

Pharmaceutical Research (2006 - 2015); Guest Editor, 2007, for  
the special theme "Materials Engineering of Solid Dosage Forms"

Journal of Controlled Release (2006 - )

Pharmaceutics (2009 - 2014)

Services and Committees:

AAPS PDD Award Committee (2002 - 2005)

AAPS CMC Fellowship Committee (2014 -)

Professional Affiliates:

AAPS (American Associate of Pharmaceutical Scientists), 1995-  
ACS (American Chemical Society), 1996-

#### REFEREED ARTICLES

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81 (b) (4)

80 Haichen Nie, Yongchao Su, Mingtao Zhang, Yang Song, Anthony Leone, Lynne S. Taylor, Patrick J. Marsac, Tonglei Li, and Stephen R. Byrn, Solid-State Spectroscopic Investigation of Molecular Interactions between Clofazimine and Hypromellose Phthalate in

- Amorphous Solid Dispersions, Molecular Pharmaceutics, DOI: 10.1021/acs.molpharmaceut.6b00740
- 79 Wei Gao, Yan Chen, David H. Thompson, Kinam Park, and Tonglei Li, Impact of surfactant treatment of paclitaxel nanocrystals on biodistribution and tumor accumulation in tumor-bearing mice, *Journal of Controlled Release*, 237:168-176, 2016, DOI:10.1016/j.jconrel.2016.07.015
- 78 Sihui Long, Mingtao Zhang, Panpan Zhou, Faquan Yu, Sean Parkin, and Tonglei Li Tautomeric Polymorphism of 4-Hydroxynicotinic Acid, *Crystal Growth & Design*, DOI:10.1021/acs.cgd.5b01639
- 77 Haichen Nie, Huaping Mo, Mingtao Zhang, Yang Song, Ke Fang, Lynne S. Taylor, Tonglei Li, and Stephen R. Byrn, Investigating the Interaction Pattern and Structural Elements of a Drug-Polymer Complex at the Molecular Level, *Molecular Pharmaceutics*, 12:2459-2468, 2015, DOI: 10.1021/acs.molpharmaceut.5b00162
- 76 Yan Chen, and Tonglei Li, Cellular Uptake Mechanism of Paclitaxel Nanocrystals Determined by Confocal Imaging and Kinetic Measurement, *AAPS Journal*, 17:1126-1134, 2015, DOI:10.1208/s12248-015-9774-0
- 75 Yi Lu, Yan Chen, Richard A. Gemeinhart, Wei Wu, and Tonglei Li, Developing Nanocrystals for Cancer Treatment, *Nanomedicine*, 10:2537-2552, 2015, DOI: 10.2217/nnm.15.73
- 74 Matthew j. Swadley, Panpan Zhou, and Tonglei Li, Reactivity of triacetone triperoxide and diacetone diperoxide: Insights from nuclear Fukui function, *Frontiers of Chemical Science and Engineering*, 9:114-123, 2015, DOI: 10.1007/s11705-015-1507-5
- 73 Sihui Long, Panpan Zhou, Sean Parkin, and Tonglei Li, Polymorphism and Solid-to-Solid Phase Transition of a Simple Organic Molecule, 3-Chloroisonicotinic Acid, *CrystEngComm*, 17:2389-2397, 2015, DOI: 10.1039/c4ce02563f
- 72 Sihui Long, Panpan Zhou, Kathryn L. Theiss, Maxime A. Siegler, and Tonglei Li, Solid-State Identity of 2-Hydroxynicotinic Acid and Its Polymorphism, *CrystEngComm*, 2015, DOI: 10.1039/c4ce02290d
- 71 Mingtao Zhang and Tonglei Li, Intermolecular Interactions in Organic Crystals: Gaining Insight from Electronic Structure Analysis by Density Functional Theory, *CrystEngComm*, 16:7162-7171, 2014, DOI: 10.1039/c4ce00411f
- 70 Alessandra Mattei, and Tonglei Li, Solution Chemistry and Its Implication on Nucleation of Conformational Polymorphs: A Computational Study of Tolfenamic Acid by Explicit Solvation, *Crystal Growth & Design*, 14:2709-2713, 2014, DOI:10.1021/cg5000815
- 69 Xi Lu, Yawei Zhang, Mingtao Zhang, Tonglei Li, The Effect of Substituents on the Hydrogenation of an Aldehyde Catalyzed by Knölker's Catalyst, *Journal of Organometallic Chemistry*, 749:69-74, 2014

- 68 Ying Lu, Zhaohui Wang, Tonglei Li, Helen McNally, Kinam Park, and Michael Sturek, Development and evaluation of transferrin-stabilized paclitaxel nanocrystal formulation, *Journal of Controlled Release*, 176:76-85, 2014
- 67 Hua Zhang, Xueqing Wang, Wenbing Dai, Richard A. Gemeinhart, Qiang Zhang, and Tonglei Li, Pharmacokinetics and Treatment Efficacy of Metastatic Lung Cancer by Camptothecin Nanocrystals, *Molecular Pharmaceutics*, 11:226-233, 2014
- 66 Sihui Long, Panpan Zhou, Sean Parkin, and Tonglei Li, From Competition to Commensuration by Two Major Hydrogen-Bonding Motifs, *Crystal Growth & Design*, 14:27-31, 2014
- 65 Christin P. Hollis, Heidi L. Weiss, B. Mark Evers, Richard A. Gemeinhart, and Tonglei Li, In Vivo Investigation of Hybrid Paclitaxel Nanocrystals with Dual Fluorescent Probes for Cancer Theranostics, *Pharmaceutical Research*, 31:1450-1459, 2014, DOI:10.1007/s11095-013-1048-x
- 64 Xi Lu, Yawei Zhang, Peng Yun, Mingtao Zhang, and Tonglei Li, The Mechanism for the Hydrogenation of Ketones Catalyzed by Knölker's Iron-Catalyst, *Organic & Biomolecular Chemistry*, 11:5264-5277, 2013
- 63 Alessandra Mattei, Xiaonan Mei, Anne-Frances Miller, and Tonglei Li, Pre-Nucleation Self-Association of Tolfenamic Acid: Solution Chemistry and Implication on Polymorph Formation, *Crystal Growth & Design*, 13:3303-3307, 2013
- 62 Christin P. Hollis, Heidi L. Weiss, Markos Leggas, B. Mark Evers, Richard A. Gemeinhart, and Tonglei Li, Biodistribution and Bioimaging Studies of Hybrid Paclitaxel Nanocrystals: Lessons Learned of the EPR Effect and Image-Guided Drug Delivery, *Journal of Controlled Release*, 172:12-21, 2013
- 61 Panpan Zhou, Paul W. Ayers, Shubin Liu, and Tonglei Li, Local Reactivity Descriptors Based on Natural Bond Orbital Occupancy: Natural Orbital Fukui Functions (NOFFs) and their applications in the reaction mechanisms of addition reactions, *Journal of Chemical Physics*, 14:9890-9896, 2012, DOI:10.1039/C2CP40488E
- 60 Alessandra Mattei and Tonglei Li, Polymorph Formation and Nucleation Mechanism of Tolfenamic Acid in Solution: An Investigation of Pre-Nucleation Solute Association, *Pharmaceutical Research*, 29:460-470, 2012, DOI:10.1007/s11095-011-0574-7
- 59 Tonglei Li, Alessandra Mattei, and Panpan Zhou, Electronic Origin of Pyridinyl N Being A Better Hydrogen-Bonding Acceptor Than Carbonyl O, *CrystEngComm*, 13:6356-6360, 2011, DOI:10.1039/C1CE05967J
- 58 Rongsheng Zhao, Christin P. Hollis, Hua Zhang, Lili Sun, Richard A. Gemeinhart, and Tonglei Li, Hybrid Nanocrystals: Achieving Concurrent Therapeutic and Bioimaging Functionalities Toward

- Solid Tumors, *Molecular Pharmaceutics*, 8:1985-1991, 2011, DOI:10.1021/mp200154k
- 57 Julio Gutierrez, Rodney Eisenberg, Gabrielle Herrensmitth, Thomas Tobin, Tonglei Li, and Sihui Long, Solvatomorphism in (*E*)-2-(2,6-dichloro-4-hydroxybenzylidene)hydrazinecarboximidamide, *Acta Crystallographica C*, 67:o310-o314, 2011, DOI: 10.1107/S0108270111023845
- 56 Hua Zhang, Christin P. Hollis, Qiang Zhang, and Tonglei Li, Preparation and Antitumor Study of Camptothecin Nanocrystals, *International Journal of Pharmaceutics*, 415:293-300, 2011, DOI: 10.1016/j.ijpharm.2011.05.075
- 55 Alessandra Mattei and Tonglei Li, Interplay between Molecular Conformation and Intermolecular Interactions in Conformational Polymorphism: A Molecular Perspective from Electronic Calculations of Tolfenamic Acid (invited), *International Journal of Pharmaceutics*, 418:179-186, 2011, DOI: 10.1016/j.ijpharm.2011.04.062
- 54 Sihui Long and Tonglei Li, Phase Transition from Two  $Z' = 1$  Forms to A  $Z' = 2$  Form of A Concomitant Conformational Polymorphic System, *Crystal Growth & Design*, 11:414-421, 2011, DOI: 10.1021/cg101009g
- 53 Paul W. Ayers, Shubin Liu, and Tonglei Li, Stability Conditions for Density Functional Reactivity Theory: An Interpretation of the Total Local Hardness, *Physical Chemistry Chemical Physics*, 13:4427-4433, 2011
- 52 Julio Gutierrez, Rodney Eisenberg, Gabrielle Herrensmitth, Thomas Tobin, Tonglei Li, and Sihui Long, Polymorphism in 2-((4-hydroxy-2,6-dimethylphenyl)amino)-5,6-dihydro-4*H*-1,3-thiazin-3-ium Chloride, *Acta Crystallographica C*, 66:o593-o595, 2010, DOI: 10.1107/S0108270110045099
- 51 Peter Guerrieri, Alfred C. F. Rumondor, Tonglei Li, and Lynne S. Taylor, Analysis of Relationships between Solid-State properties, Counterion and Developability of Pharmaceutical Salts, *AAPS PharmSciTech*, 11:1212-1222, 2010, DOI: 10.1208/s12249-010-9499-4
- 50 Sihui Long and Tonglei Li, Enforcing Molecule's  $\pi$ -Conjugation and Consequent Formation of the Acid-Acid Homosynthon over the Acid-Pyridine Heterosynthon in 2-Anilinonicotinic Acids, *Crystal Growth & Design*, 10:2465-2469, 2010, DOI: 10.1021/cg100227s
- 49 Timothy McPherson, Rahul Manek, William Kolling, Sihui Long, and Tonglei Li, Physical Characterization of 1,3-Dipropyl-8-Cyclopentylxanthine (CPX), *AAPS PharmSciTech*, 11:720-728, 2010, DOI: 10.1208/s12249-010-9436-6
- 48 Sihui Long, Kathryn L. Theiss, Alessandra Mattei, Charles D. Loftin, and Tonglei Li, Solid-State Properties of the Cyclooxygenase-1-Selective Inhibitor, SC-560, *AAPS PharmSciTech*, 11:485-488, 2010, DOI: 10.1208/s12249-010-9407-y

- 47 Sihui Long and Tonglei Li, Controlled Formation of the Acid-Pyridine Heterosynthon over the Acid-Acid Homosynthon in 2-Anilininicotinic Acids, *Crystal Growth & Design*, 9:4993-4997, 2009, DOI: 10.1021/cg900786b
- 46 Paul W. Ayers, Shubin Liu, and Tonglei Li, Chargephilicity and Chargephobicity: Two New Reactivity Indicators for External Potential Changes from Density Functional Reactivity Theory, *Chemical Physics Letters*, 480:318-321, 2009, DOI:10.1016/j.cplett.2009.08.067
- 45 Shubin Liu, Tonglei Li, and Paul W. Ayers, Potentialphilicity and Potentialphobicity: Reactivity Indicators for External Potential Changes from Density Functional Reactivity Theory, *Journal of Chemical Physics*, 131:114106, 2009, DOI:10.1063/1.3231687
- 44 Sihui Long, Kathryn L. Theiss, Tonglei Li, and Charles D. Loftin, Crystal Structure of the Cyclooxygenase-1-Selective Inhibitor, SC-560, *Acta Crystallographica E*, 65:o360, 2009, DOI:10.1107/S1600536809001779
- 43 Patrick J. Marsac, Tonglei Li, and Lynne S. Taylor, Estimation of Drug-Polymer Miscibility and Solubility in Amorphous Solid Dispersions using Experimentally Determined Interaction Parameters, *Pharmaceutical Research*, 26:139-151, 2009, DOI: 10.1007/s11095-008-9721-1
- 42 Tonglei Li, Paul W. Ayers, Shubin Liu, Matthew J. Swadley, and Clare Aubrey-Medendorp, Crystallization Force: A Density Functional Theory Concept for Revealing Intermolecular Interactions and Molecular Packing in Organic Crystals, *Chemistry - A European Journal*, 15:361-371, 2009, DOI: 10.1002/chem.200801056
- 41 Melanie R. Hauser, Lev Zhakarov, Kenneth M. Doxsee, and Tonglei Li, Polymorphism of a Simple Organic Amide, *Crystal Growth & Design*, 8:4428-4431, 2008, DOI: 10.1021/cg800171h
- 40 Sihui Long, Sean Parkin, Maxime Siegler, Arthur Cammers, Tonglei Li, Polymorphism and Phase Behaviors of 2-(Phenylamino)nicotinic Acid, *Crystal Growth and Design*, 8: 4006-4013, 2008, DOI: 10.1021/cg800123z
- 39 Christopher S. Towler, Tonglei Li, Håkan Wikström, David M. Remick, Manuel V. Sanchez-Felix, and Lynne S. Taylor, An Investigation into the Influence of Counter-ion on the Properties of Some Amorphous Organic Salts, *Molecular Pharmaceutics*, 5:946-955, 2008, DOI: 10.1021/mp8000342
- 38 Gilbert Ng, Karan Sharma, Sandra M. Ward, Melanie D. Desrosiers, Leslie A. Stephens, W. Michael Schoel, Tonglei Li, Clifford A. Lowell, Chang-Chun Ling, Matthias W. Amrein, and Yan Shi, Receptor-Independent, Direct Membrane Binding Leads to Cell Surface Lipid Sorting and Dendritic Cell Phagocytic Activities, *Immunity*, 29: 807-818, 2008, DOI: 10.1016/j.immuni.2008.09.013

- 37 Sihui Long, Sean Parkin, Maxime Siegler, Carolyn P. Brock, Arthur Cammers, Tonglei Li, The Polymorphism of an Organic System Effected by the Directionality of Hydrogen-Bonding Chains, *Crystal Growth and Design*, 8:3137-3140, 2008
- 36 Tonglei Li, *Materials Engineering of Solid-State Dosage Forms, Pharmaceutical Research*, 25:949-952, 2008
- 35 Tonglei Li, Further Understanding of the Thermal Motions of Atoms in Aspirin and Acetaminophen Crystals with Conceptual Density Functional Theory, *Crystal Growth and Design*, 8:1110-1112, 2008
- 34 Clare Aubrey-Medendorp, Matthew J. Swadley, and Tonglei Li, The Polymorphism of Indomethacin: An Analysis by Density Functional Theory Calculations, *Pharmaceutical Research*, 25:953-959, 2008
- 33 Tonglei Li, Visualizing the Locality of Intermolecular Interactions in Organic Crystals, *Journal of Molecular Graphics and Modelling*, 26:962-965, 2008
- 32 Clare Aubrey-Medendorp, Sean Parkin, and Tonglei Li, The Confusion of Indexing Aspirin Crystals, *Journal of Pharmaceutical Sciences*, 97:1361-1367, 2008
- 31 Sihui Long, Maxime Siegler and Tonglei Li, 2,4,6-Trimethylbenzenaminium chloride, *Acta Crystallographica E*, 63:o3080, 2007
- 30 Salin Gupta, Sihui Long and Tonglei Li, 6-oxo-1,6-dihydropyridine-3-carboxylic acid, *Acta Crystallographica E*, 63:o2784, 2007
- 29 Sihui Long, Sean Parkin and Tonglei Li, 3-Carboxy-2-(2,6-dimethylphenylamino)-pyridinium trifluoroacetate, *Acta Crystallographica E*, 63:o906-o907, 2007
- 28 Matthew Swadley and Tonglei Li, Reaction Mechanisms of Cyclotrimethylene Trinitramine Deciphered by Density Functional Theory, *Journal of Chemical Theory and Computation*, 3:505-513, 2007
- 27 Tonglei Li, Understanding the Polymorphism of Aspirin with Electronic Calculations, *Journal of Pharmaceutical Sciences*, 96:755-760, 2007
- 26 Sihui Long, Maxime Siegler and Tonglei Li, 6-Chloronicotinic Acid, *Acta Crystallographica E*, 63:o279-o281, 2006
- 25 Sihui Long, Maxime Siegler and Tonglei Li, 2-Oxo-1,2-dihydropyridine-3-carboxylic acid, *Acta Crystallographica E*, 62:o5664-o5665, 2006
- 24 Tonglei Li, Understanding the Large Librational Motion of the Methyl Group in Aspirin and Acetaminophen Crystals: Insights from Density Functional Theory, *Crystal Growth and Design*, 6:2000-2003, 2006

- 23 Sihui Long, Maxime Siegler and Tonglei Li, N-(3-Chloro-2-methylphenyl)-2-oxo-1,2-dihydropyridine-3-carboxamide, *Acta Crystallographica Section E*, 62:o4278-o4279, 2006
- 22 Tonglei Li and Shaoxin Feng, Empirically Augmented Density Functional Theory for Predicting Lattice Energies of Aspirin, Acetaminophen Polymorphs, and Ibuprofen Homochiral and Racemic Crystals, *Pharmaceutical Research*, 23:2326-2332, 2006
- 21 Sihui Long, Maxime Siegler and Tonglei Li, 2-(2-Isopropylanilino)pyridine-3-carboxylic acid, *Acta Crystallographica E*, 62:o4211-o4213, 2006
- 20 Shaoxin Feng and Tonglei Li, Predicting Lattice Energy of Organic Crystal by Density Functional Theory with Empirically Corrected Dispersion Energy, *Journal of Chemical Theory and Computation*, 2:149-156, 2006
- 19 Jessika Colón Soto, Carlos Peroza Meza, Wanda Caraballo, Carlos Conde, Tonglei Li, Kenneth R. Morris, and Rodolfo J. Romañach, On Line Non-Destructive Determination of Drug Content in Moving Tablets Using Near Infrared Spectroscopy, *PAT (The Journal of Process Analytical Technology)*, 2:8-15, 2005
- 18 Tonglei Li and Shaoxin Feng, Study of Crystal Packing on the Solid-State Reactivity of Indomethacin with Density Functional Theory, *Pharmaceutical Research*, 22:1964-1969, 2005
- 17 Shaoxin Feng and Tonglei Li, Understanding Solid-State Reactions with Density Functional Theory and *Ab Initio* Methods, *Journal of Physical Chemistry A*, 109:7258-7263, 2005
- 16 Tonglei Li, Shubin Liu, Shaoxin Feng, and Clare E. Aubrey, Face-Integrated Fukui Function: Understanding Wettability Anisotropy of Molecular Crystals from Density Functional Theory (Communication), *Journal of the American Chemical Society*, 127:1364-1365, 2005
- 15 Hong Wen, Tonglei Li, Kenneth R. Morris, and Kinam Park, Dissolution Study on Aspirin and alpha-Glycine Crystals, *Journal of Physical Chemistry B*, 108:11219-11227, 2004
- 14 Hong Wen, Tonglei Li, Kenneth R. Morris, and Kinam Park, How Solvents Affect Acetaminophen Etching Pattern Formation: Interaction between Solvent and Acetaminophen at the Solid/Liquid Interface, *Journal of Physical Chemistry B*, 108:2270-2278, 2004
- 13 Tonglei Li, Gerard Frunzi, Amy Donner, Candi Choi, and Kenneth R. Morris, A Statistical Support for Using Spectroscopic Methods to Validate the Content Uniformity of Solid Dosage Forms, *Journal of Pharmaceutical Sciences*, 92:1526-1530, 2003
- 12 Jennifer J. Wang, Tonglei Li, Simon D Bateman, Rober Erck, and Kenneth R. Morris, Modeling of Adhesion in Tablet Compression I. Atomic Force Microscopy and Molecular Simulation, *Journal of Pharmaceutical Sciences*, 92:798-814, 2003



- 11 Xiaoming Chen, Tonglei Li, Kenneth R. Morris and Stephen R. Byrn, Crystal Packing and Chemical Reactivity of Two Polymorphs of Flufenamic Acid with Ammonia, *Molecular Crystals and Liquid Crystals*, 381:121-131, 2002
- 10 Tonglei Li, Hong Wen, Kinam Park, and Kenneth R. Morris, How Specific Interactions between Acetaminophen and Its Additive 4-Methylacetanilide Affect Growth Morphology: Elucidation Using Etching Patterns, *Crystal Growth & Design*, 2:185-189, 2002
- 9 Tonglei Li, Kenneth R. Morris, and Kinam Park, Understanding the Formation of Etching Patterns Using a Refined Monte Carlo Simulation Model, *Crystal Growth & Design*, 2:177-184, 2002
- 8 Tonglei Li, Kenneth R. Morris, and Kinam Park, Influence of Tailor-Made Additives on Etching Patterns of Acetaminophen Single Crystals, *Pharmaceutical Research*, 18:398-402, 2001
- 7 Tonglei Li, and Kinam Park, A Monte Carlo Simulation of Grafted Poly(Ethylene Oxide) Chains, *Computational and Theoretical Polymer Science*, 11:133-142, 2001
- 6 Tonglei Li, Kenneth R. Morris, and Kinam Park, The Influence of Solvent and Crystalline Supramolecular Structure on the Formation of Etching Patterns on Acetaminophen Single Crystals. A Study with Atomic Force Microscopy and Computer Simulation, *Journal of Physical Chemistry B*, 104:2019-2032, 2000
- 5 Tonglei Li, and Kinam Park, Fractal Analysis of Pharmaceutical Granules and Powders, *Pharmaceutical Research*, 15:1222-1232, 1998
- 4 Tonglei Li, Hai-Bang Lee, and Kinam Park, Comparative Stereochemical Analysis of Glucose-Binding Proteins for Rational Design of Glucose-Specific Agents, *Journal of Biomaterials Science, Polymer Edition*, 9:327-344, 1998
- 3 Tonglei Li, Dane O. Kildsig, and Kinam Park, Computer Simulation of Molecular Diffusion in Amorphous Polymers, *Journal of Controlled Release*, 48:57-66, 1997
- 2 Tonglei Li, Shaofan Lin, and Jinbei Zhang, MouMol3D: An Interactive 3-D Molecular Building and Graphics System for PC Computers, *Selected Papers of Engineering Chemistry and Metallurgy (Chinese)*, 173-178, 1993
- 1 Tonglei Li, and Shaofan Lin, Molecular Modeling, *Journal of Computers and Applied Chemistry (Chinese)*, 9:92-98, 1992

#### PROCEEDINGS AND PRESENTATIONS

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##### Proceedings:

- 11 Christin P. Hollis, Rongsheng Zhao, Hua Zhang, Lili Sun, Barbara Knutson, and Tonglei Li, Development of Multifunctional Hybrid Nanocrystals for Cancer Therapy and Diagnosis, 2011 Controlled Release Society, Washington, DC

- 10 Sihui Long, Alessandra Mattei, and Tonglei Li, Molecular Packing in Organic Crystals: Interplay between a Molecule's Conformation and Its Intermolecular Interactions, The 2009 International Meeting on Crystal Engineering & Drug Delivery System, 2009, Tianjin, China
- 9 Tonglei Li, Christin P. Hollis, Hong Yang, and Kimberly W. Anderson, 2008 Era of Hope DOD Breast Cancer Research Program Meeting, 2008, Baltimore, MD
- 8 Yuxin Yang and Tonglei Li, Development of Novel Nanocrystals To Target Breast Cancer, 2005 Era of Hope DOD Breast Cancer Research Program Meeting, p125, 2005, Philadelphia, PA
- 7 Shaoxin Feng and Tonglei Li, Understanding Solid-State Reactions with Density Functional Theory Based Concepts and Methods, ICCOSS XVII, 2005, Los Angeles, CA
- 6 Tonglei Li and Kinam Park, Analysis of Glucose-Binding Molecules, the 25th International Symposium on Controlled Release of Bioactive Materials, p116-117, 1998, Las Vegas, NV
- 5 Tonglei Li, Dane O. Kildsig, and Kinam Park, Computer Simulation of Drug Diffusion in Amorphous Polymers, the 23rd International Symposium on Controlled Release of Bioactive Materials, p459-460, 1996, Kyoto, Japan
- 4 Tonglei Li, Dane O. Kildsig, and Kinam Park, Computer Simulation of Drug Diffusion in Amorphous Polyethylene, the 21st International Symposium on Controlled Release of Bioactive Materials, p535-536, 1994, Nice, France
- 3 Tonglei Li, and Shaofan Lin, Development of a CAMD System on PCs, the Chinese 4th Conference of Computer Chemistry, 1993, Tianjin, China
- 2 Tonglei Li, and Shaofan Lin, Stereo Display of Molecular Models for PCs, the Chinese 4th Conference of Computer Chemistry, 1993, Tianjin, China
- 1 Tonglei Li, Shaofan Lin, Jinpei Zhang, and Jinwan Shen, A Molecular Modeling and Display System for Microcomputers, the 2nd International Conference on CAD&CG, p51-53, 1991, Hangzhou, China

Presentations:

- 69 Tonglei Li, Development of Drug Nanocrystals, AIChE Midwest Regional Conference, March 4, 2016 Chicago
- 68 Arjun Kalra and Tonglei Li, SSNMR and Computational Study of Phase Transition Of Structurally Similar Compounds, AAPS Annual Meeting, 2014, San Diego (*poster*)
- 67 Arjun Kalra and Tonglei Li, SSNMR and Computational Study of Phase Transition Of Structurally Similar Compounds, AAPS Annual Meeting, 2013, San Antonio (*poster*)

- 66 Zhaohui Wang, Yan Chen, Christin Hollis, Jennifer Chough, and Tonglei Li, Hybrid Nanocrystals for Cancer Theranostics, Purdue University Center for Cancer Research Retreat, 2013, Purdue University (*poster*)
- 65 Arjun Kalra and Tonglei Li, Development of an NMR Method to Probe the Conformational Distribution of Molecules in the Solid State, CPPR Meeting, 2013, Purdue University (*poster*)
- 64 Iris Archer, and Tonglei Li, In Vitro Testing of Paclitaxel Nanocrystals in Cancer Cell Lines, SURF Presentations, 2013, Purdue University (*podium*)
- 63 Nick Turner, Tonglei Li, and Mingtao Zhang, Investigating Intermolecular Interactions in Crystalline Aspirin Using Conceptual Density Functional Theory, SURF Presentations, 2013, Purdue University (*poster*)
- 62 Zhiwei Liao, Mingtao Zhang, and Tonglei Li, Investigation of Major Intermolecular Interactions in 7,8-dihydrobenzo(k)phenanthridin-6(5H)-one Crystal Using Quantum Calculations and Crystallographic Visualization Programs, SURF Presentations, 2013, Purdue University (*poster*)
- 61 KoanHee Rim, Zhaohui Wang, and Tonglei Li, Testing Cytotoxicity of Nanocrystal Drug Delivery Systems In Vitro, DURi Presentations, 2013, Purdue University (*poster*)
- 60 Arjun Kalra and Tonglei Li, Mechanistic Investigation of the Molecular Basis of Crystallization Tendency of Amorphous Melts, AAPS Annual Meeting, 2012, Chicago (*poster*)
- 59 Arjun Kalra and Tonglei Li, Mechanistic Investigation of the Molecular Basis of Crystallization Tendency of Amorphous Melts, 44th Annual Pharmaceutics Graduate Student Research Meeting (PGSRM), Omaha, Nebraska, 2012 (*poster*)
- 58 Alessandra Mattei and Tonglei Li, Self-Assembly During Pre-nucleation and Its Impact on Polymorphic Formation, Gordon Research Conference on Crystal Engineering, 2012, Waterville Valley, NH (*poster*)
- 57 Alessandra Mattei and Tonglei Li, Investigating Solution Chemistry of Tolfenamic Acid with Molecular Dynamics and Quantum Mechanics/Molecular Mechanics, AAPS Annual Meeting, 2011, Washington DC (*poster*)
- 56 Alessandra Mattei, Xiaonan Mei, Anne-Frances Miller, and Tonglei Li, Solution NMR Investigation of Molecular Conformation and Self-Association of Tolfenamic Acid and Its Nucleation Mechanism, AAPS Annual Meeting, 2011, Washington DC (*poster*)
- 55 Christin P. Hollis, Allan Dozier, Barbara Knutson, and Tonglei Li, Preparation and Characterization of Multimodal Hybrid Nanocrystals of Camptothecin and Gold, AAPS Annual Meeting, 2011, Washington DC (*poster*)

- 54 Christin P. Hollis, Rongsheng Zhao, Hua Zhang, Richard A. Gemeinhart, and Tonglei Li, Development of Multifunctional Hybrid Nanocrystals for Cancer Therapy and Diagnosis, AAPS Annual Meeting, 2011, Washington DC (*poster*)
- 53 Christin P. Hollis, Joseph Valentino, Peter Rychahou, Mark Evers, and Tonglei Li, Nanocrystals of PI3K and MEK Inhibitors for the Therapy of Colon Cancer, AAPS Annual Meeting, 2011, Washington DC (*poster*)
- 52 Alessandra Mattei, Xiaonan Mei, Anne-Frances Miller, and Tonglei Li, NMR Study of Pre-nucleation Self-association, 43rd Annual Pharmaceutics Graduate Student Research Meeting (PGSRM), 2011, Madison, WI (*podium*)
- 51 Alessandra Mattei and Tonglei Li, Investigation of a Relationship between Molecular Conformation and Intermolecular Interactions: A Case of Tolfenamic Acid, AAPS Annual Meeting, 2010, New Orleans, LA (*poster*)
- 50 Christin P. Hollis, Emily Raetz, and Tonglei Li, Using Surface Energy of Eutectic Melt to Understand the Interaction between Eutectic Constituents, AAPS Annual Meeting, 2010, New Orleans, LA (*poster*)
- 49 Ting Wang, Carl R. Wassgren, Kristine Alston, Tonglei Li, Prabir K. Basu, Linas Mockus, and Stephen W. Hoag, Key Issues in Understanding and Predicting Excipient Properties and Functionality, AAPS Annual Meeting, 2010, New Orleans, LA (The abstract wins 2010 Regulatory Science Section of AAPS Outstanding Contributed Paper Award) (*poster*)
- 48 Tonglei Li, Paul Ayers, and Shubin Liu, Developing DFT Concepts for Characterizing Intermolecular Interactions in Organic Crystals, ACS Annual Meeting, 2010, Boston, MA (*poster*)
- 47 Sihui Long and Tonglei Li, Synthesis and Polymorphism of Clonixin Analogs, 42nd Annual Pharmaceutics Graduate Student Research Meeting (PGSRM), 2010, Columbus, OH (*podium*)
- 46 Alessandra Mattei and Tonglei Li, Conformational Polymorphism of Tolfenamic Acid: An Analysis by Electronic Calculations, 42nd Annual Pharmaceutics Graduate Student Research Meeting (PGSRM), 2010, Columbus, OH (*poster*)
- 45 Tonglei Li, Shubin Liu, and Paul Ayers, Understanding Intermolecular Interactions with Density Functional Theory, Gordon Research Conference on Crystal Engineering, 2010, Waterville Valley, NH (*poster*)
- 44 Sihui Long and Tonglei Li, Selective Formation of Acid-Pyridine Catemer Motifs in 2-Anilinonicotinic Acids, AAPS Annual Meeting, 2009, Los Angeles, CA (*poster*)
- 43 Alessandra Mattei and Tonglei Li, Mechanistic Study of Polymorphic Phase Transformation, AAPS Annual Meeting, 2009, Los Angeles, CA (*poster*)

- 42 Alessandra Mattei and Tonglei Li, Polymorph Selection: A Study of Tolfenamic Acid, 41st Annual Pharmaceuticals Graduate Student Research Meeting (PGSRM), 2009, West Lafayette, IN (*poster*)
- 41 Sihui Long and Tonglei Li, Selective Formation of Acid-Pyridine Catemer Motif in 2-Anilinic Nicotinic Acids, 41st Annual Pharmaceuticals Graduate Student Research Meeting (PGSRM), 2009, West Lafayette, IN (*podium*)
- 40 Sihui Long, Kathryn L. Theiss, and Tonglei Li, pH and Solvent Effects on the Packing Polymorphism of 2-Hydroxynicotinic Acid, AAPS Annual Meeting, 2008, Atlanta, GA (*poster*)
- 39 Alessandra Mattei, Sihui Long, and Tonglei Li, Chemical Structure and Crystal Growth: A Study of Diarylamines, AAPS Annual Meeting, 2008, Atlanta, GA (*poster*)
- 38 Christin P. Hollis, Alessandra Mattei, and Tonglei Li, A Surface Energy Model of Eutectic Formation, AAPS Annual Meeting, 2008, Atlanta, GA (*poster*) - *Travel Award by AAPS*
- 37 Sihui Long and Tonglei Li, A Polymorphic System Determined by the Directionality of Hydrogen Bonds, Annual Meeting of American Crystallographic Association, 2008, Knoxville, TN (*poster*)
- 36 Sihui Long and Tonglei Li, Disappearing Polymorphs, Midwest Organic Solid State Chemistry Symposium XIX, 2008, Manhattan, KS (*podium*)
- 35 Clare Aubrey-Medendorp and Tonglei Li, Confusion in Indexing Aspirin Crystals, Midwest Organic Solid State Chemistry Symposium XIX, 2008, Manhattan, KS (*podium*)
- 34 Clare Aubrey-Medendorp, Christin P. Hollis and Tonglei Li, A Novel Method for Measuring Surface Energy with Atomic Force Microscopy, AAPS Annual Meeting, 2007, San Diego (*poster*)
- 33 Christin P. Hollis, Clare Aubrey-Medendorp and Tonglei Li, Surface Energy Measurement of Acetaminophen Crystals with AFM, AAPS Annual Meeting, 2007, San Diego (*poster*)
- 32 Salin Gupta, Sihui Long and Tonglei Li, Studying the Solvent Effect on Polymorph Formation of 6-Hydroxynicotinic Acid, AAPS Annual Meeting, 2007, San Diego (*poster*)
- 31 Sihui Long and Tonglei Li, Polymorphism of 4-Chloronicotinic Acid Derivatives, AAPS Annual Meeting, 2007, San Diego (*poster*)
- 30 Clare Aubrey-Medendorp and Tonglei Li, Developing an AFM Method for Determining Surface Energy of Organic Crystals, Midwest Organic Solid State Chemistry Symposium XVIII, 2007, Lexington, KY (*podium*)
- 29 Sihui Long and Tonglei Li, Polymorphism and Phase Transition of 2-(Phenylamino)nicotinic Acid, Midwest Organic Solid State Chemistry Symposium XVIII, 2007, Lexington, KY (*podium*)

- 28 Clare Aubrey-Medendorp and Tonglei Li, Surface Energy Evaluation with Atomic Force Microscopy, AAPS Annual Meeting, 2006, San Antonio, TX (*poster*)
- 27 Clare Aubrey-Medendorp, Matthew Swadley and Tonglei Li, Electronic Studies of the Polymorphism of Organic Crystals with Density Functional Theory, AAPS Annual Meeting, 2006, San Antonio, TX (*poster*)
- 26 Yuxin Yang and Tonglei Li, Characterization of Eutectic Mixture Formed by Grinding, AAPS Annual Meeting, 2006, San Antonio, TX (*poster*)
- 25 Zhan Wang and Tonglei Li, Preparation of L-Cysteine Polymorphs, AAPS Annual Meeting, 2006, San Antonio, TX (*poster*)
- 24 Matthew Swadley, Clare Aubrey-Medendorp and Tonglei Li, Understanding Conformational Polymorphism with Electronic Calculations and Density Functional Theory-Based Concepts, Midwest Organic Solid State Chemistry Symposium XVII, 2006, Iowa City, IA (*podium*)
- 23 Yuxin Yang and Tonglei Li, Preparation of Eutectic Mixtures by Grinding, Midwest Organic Solid State Chemistry Symposium XVII, 2006, Iowa City, IA (*podium*)
- 22 Clare Aubrey-Medendorp and Tonglei Li, Investigating Surface Free Energy of Single Aspirin Crystals using the Atomic Force Microscopy, Midwest Organic Solid State Chemistry Symposium XVI, 2006, Iowa City, IA (*podium*)
- 21 Shaoxin Feng and Tonglei Li, Prediction of Lattice Energies of Drug Crystals with Density Functional Theory and Empirical Corrections of Dispersion Energy, AAPS Annual Meeting, 2005, Nashville, TN (*poster*)
- 20 Clare Aubrey and Tonglei Li, Investigation of Surface Energy of Single Aspirin Crystals with Contact Angle and Atomic Force Microscopy, AAPS Annual Meeting, 2005, Nashville, TN (*poster*)
- 19 Shaoxin Feng and Tonglei Li, Understanding Reactivity Difference of Indomethacin Polymorphs with Density Functional Theory-based Concepts, Midwest Organic Solid State Chemistry Annual Meeting XV, 2005, West Lafayette, IN (*podium*)
- 18 Shaoxin Feng and Tonglei Li, Calculation of Lattice Energies of Molecular Crystals with Density Functional Theory and Empirical Corrections of the Dispersion Energy, Midwest Organic Solid State Chemistry Annual Meeting XV, 2005, West Lafayette, IN (*podium*)
- 17 Shaoxin Feng and Tonglei Li, Understanding Solid-State Reactions with Density Functional Theory and *Ab Initio* Methods, AAPS Annual Meeting, 2004, Baltimore, MD (*poster*)
- 16 Clare E. Aubrey and Tonglei Li, Surface Energy Measurement with Atomic Force Microscopy, AAPS Annual Meeting, 2004, Baltimore, MD (*poster*)

- 15 Clare E. Aubrey and Tonglei Li, Surface Energy Evaluation with Atomic Force Microscopy, Nanotechnology Conference, 2003, Louisville, KY (*poster*)
- 14 Shaoxin Feng, Clare E. Aubrey, Shubin Liu and Tonglei Li, Analysis of the Anisotropic Wettability of Aspirin Single Crystals with Ab Initio Calculation, AAPS Annual Meeting, 2003, Salt Lake City, UT (*poster*)
- 13 Tonglei Li, Kenneth Morris and Kinam Park, Appearance of new growth faces of acetaminophen crystals and elucidation with possible dissolution mechanisms, AAPS Annual Meeting, 2002, Toronto, Canada (*poster*)
- 12 Tonglei Li, Kenneth Morris and Kinam Park, Influence of tailor-made additives on etching patterns of acetaminophen single crystals: Understanding through modeling and Monte Carlo simulation, AAPS Annual Meeting, 2001, Denver, CO (*poster*)
- 11 Hong Wen, Tonglei Li, Kenneth Morris and Kinam Park, Characterization of etching patterns of crystal surfaces, AAPS Annual Meeting, 2001, Denver, CO (*poster*)
- 10 Tonglei Li, Kenneth Morris and Kinam Park, Using the etching pattern to understand the interaction mechanism between tailor-made additives and the crystal surface, Midwest Organic Solid State Chemistry Annual Meeting, 2001, Lincoln, NE (*podium*)
- 9 Tonglei Li, Kenneth Morris and Kinam Park, Influence of Tailor-Made Additives on Etching Patterns of Acetaminophen Single Crystals, AAPS Annual Meeting, 2000, Indianapolis, IN (*poster*)
- 8 Tonglei Li, Kenneth Morris and Kinam Park, Influence of Tailor-Made Additives on the Formation of Etching Patterns of Acetaminophen Single Crystals, Midwest Organic Solid State Chemistry, 2000, West Lafayette, IN (*podium*)
- 7 Tonglei Li, Kenneth Morris and Kinam Park, A Study of Etching Mechanism Of Acetaminophen Single Crystals With Atomic Force Microscopy And Computer Simulation, AAPS Annual Meeting, 1999, New Orleans, LA (*poster*)
- 6 Tonglei Li, Kenneth Morris and Kinam Park, Fractal and Simulation Studies of Acetaminophen during Dissolution, AAPS Annual Meeting, 1998, San Francisco, CA (*poster*)
- 5 Kinam Park and Tonglei Li, Fractal Analysis of Pharmaceutical Particles, Conference on Pharmaceutical Science and Technology, 1998, Dallas, TX (*podium*)
- 4 Tonglei Li, and Kinam Park, Fractal Analysis of Pharmaceutical Solid Particles, 1997 AAPS Annual Meeting, 1997, Boston, MA (*poster*)
- 3 Tonglei Li, and Kinam Park, Monte Carlo Simulation of Surface Grafted PEO Chains, the 29th International Biomaterials Symposium, 1997, New Orleans, LA (*poster*)

- 2 Tonglei Li and Kinam Park, Monte Carlo Simulation of Grafted Polymer Chains on Surface, Pharmaceuticals Graduate Student Research Meeting, 1995, Ann Arbor, MI (*podium*)
- 1 Tonglei Li, Dane O. Kildsig and Kinam Park, Monte Carlo Simulation of Solid Dissolution Process and Fractal Analysis of the Surface Roughness, Pharmaceuticals Graduate Student Research Meeting, 1994, Omaha, NE (*podium*)

#### BOOK CHAPTERS

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- 4 Christin P. Hollis, Rongsheng Zhao, and Tonglei Li, Hybrid Nanocrystal as a Versatile Platform for Cancer Theranostics, in Biomaterials for Cancer Therapeutics, Kinam Park (ed), Woodhead Publishing Ltd, 2014
- 3 Christin P. Hollis and Tonglei Li, Nanocrystals: Production, Characterization, and Application for Cancer Therapy, in Nanoparticulate Drug Delivery Systems: Strategies, Technologies, and Applications, Yoon Yeo (ed), John Wiley and Sons, 2013
- 2 Jin Ho Lee, Tonglei Li, and Kinam Park, Solvation Interactions for Protein Adsorption to Biomaterial Surfaces, in Water in Biotechnological Surface Science, Marco Morra (ed), John Wiley and Sons, p127-146, 2001
- 1 Kinam Park, Aiman Obaidat, Tonglei Li, and Haesun Park, Future of Glucose Sensing and Insulin Delivery: A Point of View, in Advances in Polymeric Biomaterials Science, T. Akaike, T. Okano, M. Akashi, M. Terano and N. Yui (eds), CMC Co., Ltd., Tokyo, p465-487, 1997

#### BOOK REVIEW

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- 4 Tonglei Li, Molecular Conceptor. Drug Design Courseware, Synergix Ltd., 2002. Pharmaceutical Research, 20:2046, 2003
- 3 Tonglei Li, Computational Methods for Protein Folding, Richard A. Friesner (ed), John Wiley & Sons, New York, 2002, Pharmaceutical Research, 19:1078, 2002
- 2 Tonglei Li, Supervised and Unsupervised Pattern Recognition, Evangelia Micheli-Tzanakou, CRC Press LLC., Boca Raton, 2000, Pharmaceutical Research, 17:1440-1441, 2000
- 1 Tonglei Li and Kinam Park, Fractal Aspects of Materials, F. Family, P. Meakin, B. Sapoval, and R. Wood (eds.), Materials Research Society, Pittsburgh, 1995, Pharmaceutical Research, 14:551, 1997

#### PATENTS

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1 Tonglei Li, Hybrid Nanocrystals for Drug Delivery, Bioimaging, and Radiotherapy, filed 2006, approved 2015

#### INVITED TALKS

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- 56 Locality of Intermolecular Interactions in Organic Crystals, 7th European Charge Density Meeting, June 26, Warsaw, Poland
- 55 Solution Chemistry of Tolfenamic Acid, 3<sup>rd</sup> David Grand Symposium, June 21, 2014, Minneapolis, MN
- 54 Intermolecular Interactions of Pharmaceutical Solids, 48th Annual Pharmaceutics Graduate Student Research Meeting, June 18, 2016, Kansas City
- 53 Development of Drug Absorption Model, 4<sup>th</sup> DHD2 Symposium, Purdue University, April 11, 2016, West Lafayette, IN
- 52 Pharmaceutical Crystals, Shanghai Institute of Materia Medica, March 15, 2016, Shanghai, China
- 51 What Concomitant Polymorphism Can Tell Us about Nucleation Mechanism, 20<sup>th</sup> Larson Workshop, October 5, 2015, Philadelphia, PA
- 50 Digital Human for Drug Development, Korea Institute of Science and Technology, May 28, 2015, Seoul, Korea
- 49 Drug Nanocrystal Development and Crystal Engineering, Center of Crystallization, Tianjin University, May 26, 2015, Tianjin, China
- 48 Development of Nanocrystals for Cancer Therapy, Peck Symposium, Feb 27, 2015, West Lafayette, IN
- 47 Development of Digital Mouse, 2<sup>nd</sup> DHD2 Symposium, February 24, 2015, West Lafayette, IN
- 46 Nanocrystals for Drug Delivery, Second Military Medical University, January 13, 2015, Shanghai, China
- 45 Pharmaceutical Crystalline Materials: Challenges and Our Studies, Shanghai University of Traditional Chinese Medicine, January 8, 2015, Shanghai, China
- 44 Development of Nanocrystals for Cancer Therapy, Wuhan University of Technology, September 21, 2014, Wuhan, China
- 43 Nanocrystals for Drug Delivery, Chinese Pharmaceutics Conference, September 19, 2014, Changsha, China
- 42 Locality of Intermolecular Interaction, 3<sup>rd</sup> Gordon Research Conference on Crystal Engineering, June 2, 2014 Waterville Valley, NH
- 41 Interplay between Conformation and Intermolecular Interaction, 2<sup>nd</sup> David Grand Symposium, May 18, 2014, Minneapolis, MN
- 40 Nanocrystals for Drug Delivery, Eli Lilly, September 30, 2013, Indianapolis, Indiana

- 39 Nanocrystals for Drug Delivery, Boehringer Ingelheim, August 8, 2013, Danbury, Connecticut
- 38 Crystal Structure Prediction: The Challenge and Our Approach, Computational Science & Engineering at Purdue University, February 27, 2013, West Lafayette, IN
- 37 Hybrid Nanocrystal as a Versatile Platform for Cancer Theranostics, Minisymposium of Cancer Therapy at Purdue University, February 1, 2013, West Lafayette, IN
- 36 Crystal Engineering, ISPE Purdue Local Chapter, November 6, 2012, West Lafayette, IN
- 35 Interconnectivity and Interdependency between Conformation and Intermolecular Interaction, Eli Lilly Co., October 30, 2012, Indianapolis, IN
- 34 Crystal Engineering, ISPE Great Lake Symposium, September 29, 2012, Indianapolis, IN
- 33 Hybrid Nanocrystals for Cancer Theranostics, The 6th International Symposium on Intelligent Drug Delivery System, March 16, 2012, Seoul, Korea
- 32 Formation of Organic Crystal Polymorphs, Chemistry Department, Nankai University, March 12, 2012, Tianjin, China
- 31 Pre-Nucleation and Polymorph Formation, The 9<sup>th</sup> Annual Garnet E. Peck Symposium, October 20, 2011, West Lafayette, IN
- 30 Surface Energy and Its Measurement, Bristol-MyersSquibb, Materials Science, June 9, 2011, New Brunswick, NJ
- 29 Conformational Polymorphism: Insight from Electronic Calculation, Department of Pharmaceutical Sciences, University of Michigan, March 16, 2011, Ann Arbor, MI
- 28 Molecular Packing and Phase Transition of Diarylamines: Insight from Electronic Calculation, Department of Industry and Physical Pharmacy, Purdue University, December 20, 2010, West Lafayette, IN
- 27 Pre-nucleation in Crystallization of Polymorphs, 2010 David Grant Symposium, June 4, 2010, Minneapolis, MN
- 26 Interplay Between Molecule's Conformation and Intermolecular Interaction, Bristol-MyersSquibb, Biopharmaceutics R&D, March 11, 2010, New Brunswick, NJ
- 25 Molecular Packing in Organic Crystals: Interplay between a Molecule's Conformation and Its Intermolecular Interactions, The 2009 International Meeting on Crystal Engineering & Drug Delivery System, September 6, 2009, Tianjin, China
- 24 Crystallization Force: a DFT Concept for Understanding Intermolecular Interaction and Crystal Packing, Department of Chemical Engineering, Purdue University, July 28, 2009, West Lafayette, IN

- 23 Organic Crystals, Tianjin University, October 6, 2008, Tianjin, China
- 22 Understanding Crystal Packing with Electronic Calculations, Department of Chemistry, Georgetown University, March 13, 2008, Washington DC
- 21 Physical Characterization of Particles, AAPS Arden Conference, February 3, 2008, West Point, NY
- 20 Pharmaceutical Solid-State Materials: Understanding the Polymorphism with Electronic Calculations, Peking University, October 26, 2007, Beijing, China
- 19 Crystal Packing and Intermolecular Interactions: Insights by Conceptual DFT (Density Functional Theory), Institute of Solid-State Physics, Chinese Academy of Sciences, October 18, 2007, Hefei, China
- 18 Pharmaceutical Solid-State Materials, Fudan University, October 12, 2007, Shanghai, China
- 17 Surface Energy of Organic Crystals: Evaluation with AFM, University of Wisconsin, September 21, 2007, Madison, WI
- 16 Understanding the Polymorphism of Organic Crystals, University of Kansas, September 4, 2007, Lawrence, KS
- 15 Fukui Function: A DFT Concept for Understanding the Polymorphism of Organic Crystals, Boehringer Ingelheim, June 29, 2007, Danbury, Connecticut
- 14 Using AFM to Determine Surface Energy of Organic Crystals, Ninth International Workshop on Physical Characterization of Pharmaceutical Solids, June 26, 2007, Boston, Massachusetts
- 13 Aspirin, Still Causing a Headache, Pharmaceutical Sciences Postgraduate Conference, University of Kentucky, April 20, 2007, Lexington, Kentucky
- 12 Understanding Intermolecular Interactions with Density Functional Theory, Department of Chemistry, University of Kentucky, Jan. 12, 2007, Lexington, Kentucky
- 11 Electronic Studies of the Polymorphism of Organic Crystals with Density Functional Theory, AAPS Annual Meeting, Nov. 1, 2006, San Antonio, Texas
- 10 Understanding Polymorphism of Organic Crystals, Chinese Academy of Sciences Symposium on Computational Chemistry and Parallel Software, July. 11, 2006, Zhang Jia Jie, China
- 9 Understanding Crystal Growth with AFM, AAPS Annual Meeting, Nov. 7, 2005, Nashville, Tennessee
- 8 Energetic Evaluation of Crystal Surface with Atomic Force Microscopy, Boehringer Ingelheim, Oct. 11, 2005, Danbury, Connecticut

- 7 Understanding Crystal-Solvent Interactions with DFT and HSAB, AACP Annual Meeting, July 10, 2005, Cincinnati, Ohio
- 6 Understanding Crystal Growth with Density Functional Theory and HSAB Principle, University of Illinois at Chicago, Mar. 16, 2005, Chicago, Illinois
- 5 Study of Anisotropic Wettability, AAPS Annual Meeting, Nov. 12, 2004, Baltimore, Maryland
- 4 Surface Reconstruction and Crystal Growth, Pfizer, Mar. 24, 2003, Groton, Connecticut
- 3 Crystal Engineering for Better Pharmaceutical Materials, Department of Chemical & Materials Engineering, University of Kentucky, Sept. 25, 2002, Lexington, Kentucky
- 2 What if Acetaminophen Crystals Need to Relax on the Surface, Molecular Crystallization Consortium, Apr. 17, 2002, Toronto, Canada
- 1 Fractal Analysis of Pharmaceutical Materials, Oct. 2, 1998, Kalamazoo, Michigan

#### TEACHING ACTIVITIES

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##### Primary Responsibilities (Course Coordinator):

IPPH 562 (3 credits), Introduction to Pharmaceutical Manufacture, 2013 -

PHRM 82800 (3 credits), Dosage Form I, 2012

PHR 914 (3 credits), Introduction to Pharmaceutical Sciences I, 2005 - 2011

PHR 776/778 (1 credit), Pharmaceutical Sciences Seminar, 2004 - 2005

PHR 760-010 (3 credits), Analysis of Pharmaceutical Materials, 2005, 2007, 2009, 2010, 2012

PHR 760-009 (1 credit, every semester), Review of Solid-State Chemistry Literature, 2004 - 2011

##### Secondary Responsibilities:

PHR 914, Introduction to Pharmaceutical Sciences I, 2002 - 2004 (9 hours of lectures)

PHR 760, Introduction to Pharmaceutical Sciences, 2002 - (1 hour of lecture)

PHR 622, Advanced Biopharmaceutics, 2003 (3 hours of lectures)

PHR 630, Rate Processes, 2002 (3 hours of lectures)