Bernhardt L. Trout

Department of Chemical Engineering
Massachusetts Institute of Technology
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Research Interests:

Pharmaceutical manufacturing and development research, Biopharmaceutical (protein and antibody) processes and stabilization, Pharmaceutical crystallization and separations, Multi-scale modeling, Electronic-structure calculations, Rare events simulations.

Positions:

Massachusetts Institute of Technology, Cambridge, MA

Raymond F. Baddour, ScD, (1949) Professor of Chemical Engineering, October 2014 – present
Director, SEE: Society, Engineering and Ethics, Jan., 2009 - present
Director, Novartis-MIT Center for Continuous Manufacturing, June 2007 – May 2019
Co-Chair, Chemical and Pharmaceutical Engineering Singapore-MIT Alliance Program, July 2006 – October 2014
Professor of Chemical Engineering, January 2008 – October 2014
Director, Concourse Freshman Educational Program, July 2009 – June 2012
Associate Professor of Chemical Engineering, July 2003 – December 2007
Assistant Professor of Chemical Engineering, January 1998 – July 2003

Max-Planck-Institut für Festköperforschung, Stuttgart, Germany

Post-Doctoral Researcher, 1996 – 1997
Director: Michele Parrinello

Teaching:

10.01 Ethics for Engineers, 10.02 Foundations of Principled Entrepreneurship for Engineers , 10.213: Undergraduate Thermodynamics, 10.40: Graduate Thermodynamics, 10.65: Chemical Reactor Engineering, 10.541: Kinetics of Biological and Chemical Systems, 10.37: Chemical Kinetics and Reactor Design, 10.27: Process Engineering Laboratory, 10.675: Molecular Computational Methods in Chemical Engineering, 10.491: Chemical Engineering Design Module, 10A16: Freshman Advising Seminar, 10.04J Philosophical History of Energy,

ALXN2025
IPR2023-01069

ALXN2025
IPR2019-00739

Education:

University of California, Berkeley
Ph.D. in Chemical Engineering, 1996
Thesis: Reaction Processes in ZSM-5 Zeolites Elucidated by Quantum Density Functional Theory and by Dynamic Monte Carlo
Advisors: Arup K. Chakraborty and Alexis T. Bell

Université de Paris IV
Certificat de Langue et de Civilisation Françaises, 1991

Massachusetts Institute of Technology
M.S. in Chemical Engineering Practice, 1990

Massachusetts Institute of Technology
B.S. in Chemical Engineering, 1990

Awards and Honors:

The Medicine Maker "Power List", 2019
ISCMP Co-Chair, 2018
The Medicine Maker "Power List", 2017
ISCMP Co-Chair, 2016
The Medicine Maker "Power List", 2016
AIChE Division 15 (FPBE) Plenary Speaking Award, 2015
Armenian Academy of Engineering, Foreign Member, elected 2015
The Medicine Maker "Power List", 2015
AIChE Excellence in Process Development Research Award, 2014
ISCMP Co-Chair, 2014
ISCMP Downstream Pharmaceutical Panel Chair, 2014
CCR Research Collaboration Award, 2014
Manufacturing Technology Runner-up for the Wall Street Journal Technology Innovation Award, 2012
Impact Award from the Computational Molecular Science and Engineering Forum of the AIChE (CoMSEF), 2011
ACS Plenary Lecture, 2011
AIChE Area 1A Program Chair, 2006
National Academy of Engineering participant in "Frontiers in Engineering," 2001
Henry L. and Grace Doherty Professorship, 2001 – 2003
Ford Motor Company Young Investigator Award, 2001
NSF CAREER Award, 2000 – 2004
Joseph R. Mares Junior Faculty Chair, 1998 – 2001
Max-Planck Institute Fellowship, 1996 – 1997
NSF Graduate Fellowship, 1991 – 1994

Committees/Memberships:

MIT Advisory Board for Social and Ethical Responsibilities of Computing (SERC), 2019-2020
MIT Schwarzman College of Computing Committee on Social Implications, 2019
MIT Task Force on Open Access, 2017 – 2019
Task Force on Open Access, Contracts subteam, 2017-2019
United States Pharmacopeia Expert Panel: Quality Standards for Pharmaceutical Continuous Manufacturing, 2016 – present
Molecular Systems Design & Engineering (MSDE), Royal Society of Chemistry Journal, Editorial Board Member, 2016 – present
FDA Advisory Committee for Pharmaceutical Science and Clinical Pharmacology, Consultant, 2015 – 2018
MIT Chemical Engineering Department Head Search Advisory Committee, 2015
FDA Coordination Group at MIT, 2014 – 2016
MIT Committee on Intellectual Property, 2011 – 2016
MIT Committee on the Undergraduate Program, 2006 – present
MIT Faculty Search Committee, 2006 – present
MIT Practice School Steering Committee, 2004 – 2015
ISPE Subcommittee on Pharmaceutical Manufacturing, 2010 – 2011
ISPE Subcommittee on Continuous Production, 2008
MIT Graduate Committee, 2006 – 2009
DuPont-MIT Advisory Committee, 2005 – 2007
Hottel Lecture Committee, 2004 – 2007
SMA Annual Report Committee, 2003 – 2012
Department Computer Committee, 2002 – 2007

Conferences Organization:

Co-Chair, International Symposium on Continuous Manufacturing, October 2018
Co-Chair, International Symposium on Continuous Manufacturing, September 2016
Chair, MIT Mastery of Nature Conference, May 2016
Organizing Committee, AIChE/FDA P2DM Workshop on Continuous Manufacturing, March 2016
Co-Chair, International Symposium on Continuous Manufacturing, May 2014

Scientific Publications:

203. Jensen, K., Xiang, A., Fitch, H., Alden, E., Myerson, A.S., and Trout, B.L., "Water-soluble Placebo Polymer Thin Films for Continuous Manufacturing of Tablets," *J. Appl. Polym. Sci., submitted*.

202. Badman, C., Cooney, C. L., Florence, A., Konstantinov, K., Krumme, M., Nasr, M. N., Mascia, S., Trout, B.L., "Why We Need Continuous Pharmaceutical Manufacturing and How to Make it Happen," *J. Pharm. Sci.,* **108**, 3521 (2019). **Featured Article**

201. Cloutier, T., Sudrik, C., Mody, N., Sathish, H., and Trout, B. L., "Molecular Computations of Preferential Interaction Coefficients of IgG1 Monoclonal Antibodies with Sorbitol, Sucrose, and Trehalose and the Impact of These Excipients on Aggregation and Viscosity," *Molecular Pharmaceutics,* **16**, 3657 (2019).

200. Arsiccio, A., Trout, B.L., Capozzi, L.C., Pisano, R., "Achieving Continuous Manufacturing in Lyophilization: Technologies and Approaches," *EJPB,* **142**, 265 (2019).

199. Mehrabian, H., Bellucci, M., Walsh, M., and Trout, B.L., "In Silico Analysis of the Effect of Alkyl Tail Length on Anti-Agglomerant Adsorption to Natural Gas Hydrates in Brine," *J. Phys. Chem. C,* **123**, 17239 (2019). DOI: 10.1021/acs.jpcc.9b01952.

198. Gobbo, G., Ciccotti, G., and Trout, B. L., "On computing the solubility of molecular systems subject to constraints using the extended Einstein crystal method," *J. Chem. Phys*., **150**, 201104 (2019). DOI: 10.1063/1.5099378. **Editor's Pick.**

197. Sudrik, C., Cloutier, T., Mody, N., Hasige, S. A., and Trout, B. L., "Understanding the role of preferential exclusion of sugars and polyols from native state IgG1 monoclonal antibodies and its effect on aggregation and reversible self-association," *Pharm. Res.,* **36**, UNSP 109 (2019). DOI: 10.1007/s11095-019-2642-3.

196. Chadwick, K., Chen, J., Santiso, E. and Trout, B.L. "Molecular Modeling Applications in Crystallization," Ch. 5 of Handbook of Industrial Crystallization. *Cambridge University Press, ed.* Myerson, A. S, Erdemir, D., and Lee, A., p. 136 (2019).

195. Wijethunga, T., Chen, X., Myerson, A. S., Trout, B. L., "The use of functional crystalline substrates for heterogeneous nucleation and polymorphic selection of indomethacin," *Cryst. Eng. Comm.,* **21**, 2193 (2019). DOI: 10.1039/c8ce01517a

194. Bellucci, M., Gobbo, G., Wijethunga, T., Ciccotti, G., and Trout, B. L., "Solubility of Paracetamol in Ethanol by Molecular Dynamics Using the Extended Einstein Crystal Method and Experiments", *J. Chem. Phys.,* **150**, article number 094107 (2019). DOI: 10.1063/1.5086706

193. Capozzil, L. C., Trout, B. L. Pisano, R., "From batch to continuous: freeze-drying of suspended vials for pharmaceuticals in unit-doses," *I&EC,* **58**, 1635 (2019). DOI: 10.1021/acs.iecr.8b02886

192. Cloutier, T., Sudrik, C., Sathish, H., and Trout, B. L., "Kirkwood-Buff Derived Alcohol Parameters for Aqueous Carbohydrates and their Application to Preferential Interaction Coefficient Calculations of Proteins," *J. Phys. Chem. B,* **122**, 9350 (2018). DOI 10.1021/acs.jpcb.8b07623

191. Wijethunga, T., Stojakovic, J., Bellucci, M., Chen, X., Myerson, A. S., Trout, B. L., "A general method for the identification of crystal faces using Raman spectroscopy

combined with machine learning and application to the epitaxial growth of acetaminophen," *Langmuir*, **34**, 9836 (2018). DOI 10.1021/acs.langmuir.8b01791.

190. Mehrabian, H., Bellucci, M., Walsh, M., and Trout, B.L., "Effect of Salt on Anti-Agglomerant Surface Adsorption in Natural Gas Hydrates," *J. Phys. Chem. C,* **122**, 12839 (2018). DOI: 10.1021/acs.jpcc.8b03154.

189. Bellucci, M., Walsh, M., and Trout, B.L., "Molecular Dynamics Analysis of Anti-Agglomerate Surface Adsorption in Natural Gas Hydrates," *J. Phys. Chem. C,* **122**, 2673 (2018). DOI: 10.1021/acs.jpcc.7b09573

188. Gobbo, G., Bellucci, M., Tribello, G., Ciccotti, G., and Trout, B. L., "Nucleation of molecular crystals driven by relative information entropy," *J. Chem. Theory Comput.,* **14**, 959 (2018). DOI: 10.1021/acs.jctc.7b01027

187. Puri, V., Brancazio, D., Harinith, E., Martinez, A., Desai, P. M., Jensen, K. D., Chun, J., Braatz., R. D., Myerson, A. S., Trout, B. L., " Demonstration of Pharmaceutical Tablet Coating Process by Injection Molding Technology," *Int. J. Pharm.,* **535**, 106 (2018).

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184. Puri, V., Desai, P. M., Jensen, K. D., Chun, J., Myerson, A. S., Trout, B. L., "Development of Maltodextrin Based Immediate Release Tablets using an Integrated Twin-Screw Hot Melt Extrusion and Injection Molding Continuous Manufacturing Process," *J Pharm Sci.,* **106**, 3328 (2017).

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180. Yazdanpanah, N., Testa, C., Perala, S. R. K., Jensen, K., Braatz, R., Myerson, A. S., Trout, B. L., "Continuous Heterogeneous Crystallization on Excipient Surfaces," *Crystal Growth & Design,* **17**, 3321, DOI: http://dx.doi.org/10.1021/acs.cgd.7b00297 (2017).

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177. Li, J., Tsai-ta, C. L., Trout, B. L., Myerson, A. "Continuous Crystallization of Cyclosporine: The Effect of Operating Conditions on Yield and Purity," *Crystal Growth & Design,* **17**, 1000, DOI: 10.1021/acs.cgd.6gd.6b01212 (2017).

176. Sudrik, C., Cloutier, T., Pham, P., Samra, H, and Trout, B. L., "Preferential interactions of trehalose, L-arginine and sodium chloride with therapeutically relevant IgG1 monoclonal antibodies," *mAbs*, **9**, 1155 http://dx.doi.org/10.1080/19420862.2017.1358328 (2017).

175. Reslan, M., Demir, Y. K., Trout, B. L., Chan, H. K., and Kayser, V., "Lack of Synergistic Effect of Arginine-Glutamic Acid on the Physical Stability of Spray-Dried Bovine Serum Albumin," *Pharmaceutical Development and Technology*, **22**, 785, DOI: 10.1080/10837450.2016.1185116 (2017).

174. Kayser, V., Francon, A., Pinton, H., Saluzzo, J. F., Trout, B. L., "Rational Design of Rabies Vaccine Formulation for Enhanced Stability," *Turkish Journal of Medical Sciences* **47**, 987. doi:10.3906/sag-1610-82 (2017).

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172. Padhye, N., Parks, D., Slocum, A., Trout, B. L. "Enhancing the Performance of the T-Peel Test for Thin and Flexible Adhered Laminates," *Review of Scientific Instruments,* **87**, 085111; DOI: 10.1063/1.4960172 (2016).

171. Lee, K.K.H., Sahin, Y.Z., Neeleman, R., Trout, B.L. and Kayser, V., "Quantitative Determination of the Surfactant-Induced Split Ratio for Influenza Virus by Fluorescence Spectroscopy," *Human Vaccines & Immunotherapies,* **12**, 1757, DOI: 10.1080/21645515.2016.1141846 (2016).

170. Lauer, T., Wood, G., Farkas, D., Sathish, H., Samra, H., Trout, B. L. "Molecular Investigation into the Mechanism of Non-Enzymatic Hydrolysis of Proteins and Predictive Algorithm for Susceptibility," *Biochemistry,* **55**, 23, 3315-3328, DOI: 10.1021/acs.biochem.5b01376 (2016).

169. Zhou, L., Ferguson, S., Youn, Y., Trout, B.L., Myerson, A., Braatz, R. "Mathematical Modeling and Design of Falling Film Solution Crystallization," *Crystal Growth & Design*, **55**, 5019-5029, DOI: 10.21/acs.iecr.6b0057 (2016).

168. Wood, G., Alavattam, S., Moore, J., Wang, Y. J., Trout, B. L. "Mechanistic Insights Into Radical-Mediated Oxidation of Tryptophan from ab initio Quantum Chemistry Calculations and QM/MM Molecular Dynamics Simulations," *J. Phys. Chem. A,* **120**, 18, 2926-2939, DIO: 10.1021/acs.jpca.6b02429 (2016).

167. Yu, L., Akseli, I., Allen, B, et al. "Advancing Pharmaceutical Quality: a Summary of the Second FDA/PQRI Conference," AAPS Journal, **18**, 528 (2016).

166. Yazdanpanah, N., Myerson, A., Trout, B. L. "Mathematical Modeling of Layer Crystallization on a Cold Column with Recirculation," *Industrial & Engineering Chemistry Research*, **55**, 1, 5019-5029, DOI: 10.102/acs.iecr.6b00057 (2016)

165. Li, J., Trout, B. L., Myerson, A. "Multistage Continuous Mixed-Suspension, Mixed-Product Removal (MSMPR) Crystallization with Solids Recycle," *Organic Process Research & Development*, **20**, 2, 510–516, DOI: 10.1021/acs.oprd.5b00306 (2016).

164. Agrawal, N.J., Helk, B., Kumar, S., Mody, N., Sathish, H., Samra, H., Buck, P., Li, L., Trout, B.L. "Computational Tool for the Early Screening of IgG1 Monoclonal Antibodies for their Viscosities," *mAbs,* **8**, 1, 43-48, DOI: 10.1080/19420862.2015.1099773 (2016).

163. Courtois, F., Agrawal, N., Lauer, T. M., Trout, B. L. "Rational Design of Therapeutic mAbs Against Aggregation through Protein Engineering and Incorporation of Glycosylation Motifs Applied to Bevacizumab," *mAbs,* **8**, 1, 99-112, DOI: 10.1080/1942086.2015.1112477 (2016).

162. Yazdanpanah N., Ferguson, S. T., Myerson, A., Trout, B. L., "A Novel Technique for Filtration Avoidance in Continuous Crystallization," *Crystal Growth & Design,* **16**, 1, 285–296, DOI: 10.1021/acs.cgd.5b01231 (2016).

161. Chopade, P., Sarma, B., Santiso, E., Simpson, J., Fry, J., Yurttas, N., Biermann, K., Chen, J., Trout, B.L., Myerson, A. S. "On the Connection between Nonmonotonic Taste

Behavior and Molecular Conformation in Solution: The Case of Rebaudioside-A," *J. Chem. Phys..,* **143**, 24, DOI: 10.1063/1.4937946 (2016). *Editors' Choice Article*

160. Trout, B.L., Foreward to Developability of Biotherapeutics: Computational Approaches, Edited by Sandeep Kumar and Satish Kumar Singh, CRC Press (2015).

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158. O'Mahony, M., Leung, A., Ferguson, S., Trout, B.L.; Myerson, A.S. "A Process for the Formation of Nanocrystals of Active Pharmaceutical Ingredients with Poor Aqueous Solubility in a Nanoporous Substrate," *Org. Process Res. Dev.,* **19**, 9, 1109-1118, DOI: 10.1021/op500262q (2015).

157. Courtois, F., Schneider, C., Agrawal, N.J., Trout, B.L. "Rational Design of Biobetters with Enhanced Stability", *J. Pharm. Sci.,* **104**, 8, 2433-2440*,* DOI: 10.002/jps.24520 (2015).

156. Tsai-Ta, C.L., Cornevin, J., Ferguson, S., Li, N., Trout, B.L., Myerson, A. "Control of Polymorphism in Continuous Crystallization via MSMPR Cascade Design," *Crystal Growth and Design*, **15**, 7, 3374–3382, DOI: 10.1021/acs.cgd.5gd.5b00466 (2015).

155. Sharma, M., Trout, B.L. "Effect of Pore Size and Interactions on Paracetamol Aggregation in Porous Polyethylene Glycol Diacrylate Polymers," *J. Phys Chem. B*, **119**, 25, 8135–8145, DOI: 10.1021/jp512788a (2015).

154. Yu, L. X., Akseli, I., Allen, B., Amidon, G., Bizjak, T. G., Boam, A., Caulk, M., Doleski, D., Famulare, J., Fisher, A., Furness, S., Hasselbalch, B., Havel, H., Hoag, S. W., Iser, R., Johnson, B. D., Ju, R., Katz, P., Lacana, E., Lee, S. L., Lostritto, R., McNally, G., Mehta, M., Mohan, G., Nasr, M., Nosal, R., Oates, M., O'Connor, T., Polli, J., Raju, G. K., Randazzo, G., Schwendeman, A., Selen, A., Seo, P., Shah, V., Sood, R., Thien, M. P., Tong, T., Trout, B. L., Tyner, K., Vaithiyalingam, S., VanTrieste, M., Wesdyk, R., Woodcock, J., Wu, G., Wu, L., Yu, L., Zezza, D. "Advancing Product Quality: A Summary of the Second FDA/PQRI Conference," *The AAPS Journal*, **17**, 4, 1011-1018, DOI: 10.1208/s12248-015-9754-4 (2015).

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19. Cao, Z., Anderson, B.J., Tester, J.W. and Trout, B.L., "Development and application of an *ab initio* methane-water potential for the study of phase equilibria of methane hydrates," in Accurate Description of Low-lying Electronic States and Potential Energy Surfaces, eds. Hoffmann, M.R. and Dyall, K.G., *ACS Symposium Series 828*, 2002, pp. 418-444.

18. Demurov, A., Radhakrishnan, R. and Trout, B.L., "Computations of Diffusivities in Ice and CO_2 Clathrate Hydrates via Molecular Dynamics and Monte Carlo Simulations," *J. Chem. Phys.*, **116**, 702 (2002).

17. Cao, Z., Tester, J.W., Sparks, K.A. and Trout, B.L., "Molecular Computations Using Robust Hydrocarbon-Water Potentials for Describing Hydrate Phase Equilibria," *J. Phys. Chem. B*, **105**, 10950 (2001).

16. Mantz, Y.A., Geiger, F.M., Molina, L.T., Molina, M.J. and Trout, B.L., "The Interaction of HCl with the (0001) Face of Hexagonal Ice Studied Theoretically via Car-Parrinello Molecular Dynamics," *Chem. Phys. Lett.,* **348**, 285 (2001).

15. Bazant, M. and Trout, B.L., "A method to extract potentials from the temperature dependence of Langmuir constants for clathrate-hydrates," *Physica A*, **300**, 139 (2001).

14. Lin, X., Ramer, N.J., Rappe, A.M., Hass, K.C., Schneider, W.F. and Trout, B.L., "Effect of Particle Size on the Adsorption of O and S Atoms on Pt: A Density-Functional Theory Study," *J. Phys. Chem. B*, **105**, 7739 (2001).

13. Girumescu, C.A. and Trout, B.L., "Quantum Calculations and Car-Parrinello Simulations of Processes in the Zeolite Chabazite," in *Foundations of Molecular Modeling and Simulation*, eds. Cummings, P.T., Westmoreland, P.R. and Carnahan, B., *AIChE Symposium Series*, **97** (2001).

12. Mantz, Y.A., Geiger, F.M., Molina, L.T., Molina, M.J. and Trout, B.L., "First-Principles Theoretical Study of Molecular HCl Adsorption on a Hexagonal Ice (001) Surface," *J. Phys. Chem. A*., **105**, 7037 (2001).

11. Cao, Z., Tester, J.W. and Trout, B.L., "Computation of the Methane–Water Potential Energy Hypersurface via *ab initio* Methods," *J. Chem. Phys*., **115**, 2550 (2001).

10. Trout, B.L., "Car-Parrinello Methods in Chemical Engineering: Their Scope and Potential," *Adv. Chem. Eng.*, Academic Press: San Diego, **28**, 353, (2001).

9. Trout, B.L., White, D., Suits, B.H. and Gorte, R.J., "Molecular motions of hydrogen bonded CH_3CN in CHA: Comparison of first-principles molecular dynamics simulations with results from ^1H, ^2H, and ^{13}C NMR," *J. Phys. Chem B*, **104**, 11734 (2000).

8. Mantz, Y.A., Geiger, F.M., Molina, L.T., Molina, M.J. and Trout, B.L., "First-principles molecular dynamics study of surface disordering of the (0001) face of hexagonal ice," *J. Chem. Phys.*, **113**, 10733 (2000).

7. Lau, K.K.S., Gleason, K.K. and Trout, B.L., "Thermochemistry of gas phase CF_2 reactions: a density functional theory study," *J. Chem. Phys.*, **113**, 4103 (2000).

6. Trout, B.L. and Parrinello, M., "Analysis of the dissociation of H_2O in water using first principles molecular dynamics," *J. Phys. Chem. B*, **103**, 7340 (1999).

5. Sparks, K.A., Tester, J.W., Cao, Z. and Trout, B.L., "Configurational properties of water clathrates: Monte Carlo and multidimensional integration versus the Lennard-Jones and Devonshire approximation," *J. Phys. Chem. B*, **103**, 6300 (1999).

4. Trout, B.L. and Parrinello, M., "The dissociation mechanism of H_2O in water studied by first-principles molecular dynamics," *Chem. Phys. Lett.*, **288**, 343 (1998).

3. Trout, B.L., Chakraborty, A.K. and Bell, A.T., "Diffusion and reaction in ZSM-5 studied by dynamic Monte Carlo," *Chem. Eng. Sci.*, **52**, 2276 (1997).

2. Trout, B.L., Chakraborty, A.K. and Bell, A.T., "Analysis of the thermochemistry of NO_x decomposition over CuZSM-5 based on quantum chemical and statistical mechanical calculations," *J. Phys. Chem.*, **100**, 17582 (1996).

1. Trout, B.L., Chakraborty, A.K. and Bell, A.T., "Local spin density functional theory study of copper ion-exchanged ZSM-5," *J. Phys. Chem.*, **100**, 4173 (1996).

Philosophical Publications:

2. Trout, B.L., "Quantum Mechanics and Political Philosophy" Minkov, S. Y. and Trout, Bernhardt L. (Eds.), *Mastery of Nature: Promises and Prospects* (pp. 220-232) Philadelphia, PA: University of Pennsylvania Press (2018).

1. Minkov, S. Y. and Trout, Bernhardt L. (Eds.), *Mastery of Nature: Promises and Prospects*, Philadelphia, PA: University of Pennsylvania Press (2018).

Non-Peer Reviewed Publications:

3. Livingston, A., et al. "Challenges and Directions for Green Chemical Engineering-- Role of Nanoscale Materials" in *Sustainable Nanoscale Engineering*, Elsevier, Amsterdam 2020.

2. Trout, B.L., "Foreword." *Developability of Biotherapeutics: Computational Approaches,* CRC Press, 2015.

1. Mascia, S., Trout, B.L., "Integrated Continuous Manufacturing," *Pharmaceutical Manufacturing,* December 2014, pp. 26-29.

Conference Publications:

6. Buck, P.M., Kumar, S., Wang, X., Agrawal, N.J., Trout, B.L., and Singh, S.K., "Computational Methods to Predict Biotherapeutic Protein Aggregation", *Therapeutic Proteins: Methods and Protocols, Second Edition*, Springer, Humana Press. pp. 425-451 (2012).

5. Agrawal, N.J., Lauer, T.M, Hernandez-Guzman, H., Helk, B. and Trout, B.L., "Novel computational tools could mitigate antibody aggregation", *Pharmaceutical Formulation and Quality*, (2012).

4. Radhakrishnan, R., Demurov, A., Herzog, H.J. and Trout, B.L., "Modeling the dissolution of liquid CO_2 in water under hydrate forming conditions," Proceedings of the Fourth International Conference on Gas Hydrates, Yokohama, Japan, May 2002, pp. 262- 266.

3. Cao, Z., Anderson, B., Tester, J.W. and Trout, B.L., "Computations of the thermodynamics of methane hydrates using *ab initio* data," Proceedings of the Fourth International Conference on Gas Hydrates, Yokohama, Japan, May 2002, pp. 315- 320.

2. Anderson, B., Bazant, M.Z. and Trout, B.L. "Application of an analytical method to extract molecular potentials from Langmuir curve data," Proceedings of the Fourth International Conference on Gas Hydrates, Yokohama, Japan, May 2002, pp. 418-423.

1. Radhakrishnan, R. and Trout, B.L., "Mechanism for the nucleation of CO_2 hydrate clathrates studied using a Monte Carlo based approach," Proceedings of the Fourth International Conference on Gas Hydrates, Yokohama, Japan, May 2002, pp. 494-497.

Patents:

18. "Continuous Freeze-drying Methods and Related Products." US 62/500,466, Filing Date: May 2, 2017

17. "Continuous Crystallization on Excipient Surface and Tablet Making." US 62/477253, Filing Date: 27.03.2017

16. "Core-Shell Particles for Controlled Release of Organic Material." US 62/348371, Filing Date: 23.09.2016

15. "Biocompatible Polymeric Hydrogels for Controlling Nucleation from Solution and Loading of Hydrophobic and Hydrophilic Pharmaceuticals." U.S. Patent Application: 14/575069, Filing Date: 18.12.2014

14. "Computer-Implemented Methods of Determining Protein Viscosity," U.S. Patent Application: 61/824680, PCT/US2014/038368, International Filing Date: May 16, 2014.

13. "Plasticity Induced Bonding," U.S. Patent No.: 10,213,**960**, Date of Patent: Feb. 26, 2019, PCT/US2015/031666, International Filing Date: May 20, 2015.

12. "Methods and Systems for Manufacturing a Tablet." U.S. Patent No.: 10,053,798, Date of Patent: Aug. 21, 2018, Filed: Apr. 30, 2015.

11. "Layer Processing for Pharmaceuticals." U.S. Patent No.: 9,205,089, Date of Patent: Dec. 8, 2015, Filed Apr. 27, 2012.

10. "Compositions, Methods, and Systems Relating to Controlled Crystallization and/or Nucleation of Molecular Species." U.S. Patent No.: 9,138,659, Date of Patent: Sept. 22, 2015, Filed: Aug. 23, 2011.

9. "Immunoglobulins with Reduced Aggregation.", U.S. Patent No.: 9,676,841, Date of Patent: Jun. 13, 2017, PCT/US2009/047948, International Filing Date: June 19, 2009.

8. "Immunoglobulins with Reduced Aggregation.", U.S. Patent No.: 8,747,848, Date of Patent: Jun. 10, 2014, PCT/US2009/047948, International Filing Date: June 19, 2009.

7. "HER2 and VEGF-A-binding Proteins with Enhanced Stability." U.S. Patent No.: 9,777,067, Date of Patent: Oct. 3, 2017, PCT/US2013/062108, International Filing Date: Sept. 27, 2013

6. "Methods to Identify Amino Acid Residues Involved in Macromolecular Binding and Uses Therefor." U.S Patent No.: 10,431,325, Date of Patent: Oct. 1, 2019, PCT/US2013/053499, International Filing Date: Aug. 2, 2013.

5. "Methods and Systems Relating to the Selection of Substrates Comprising Crystalline Templates for the Controlled Crystallization of Molecular Species," U.S. Patent No.: 9,822,467, Date of Patent: Nov. 21, 2017, Filing Date: Nov. 15, 2012.

4. "Dendrimer-Based Excipients for the Attenuation of Protein Aggregation," U.S. Patent No.: 9,410,142, Date of Patent: Aug. 9, 2016, PCT/US2011/060400, International Filing Date: Nov. 11, 2011.

3. "Methods for Identification of Sites for IgG Conjugation.", U.S. Patent No. 9,629,925, Date of Patent: Apr. 25, 2017, PCT/US2010/037517, International Filing Date: June 4, 2010.

2. "Methods for Identification of Sites for IgG Conjugation.", U.S. Patent No. 8,834,885, Date of Patent: Sept. 16, 2014, PCT/US2010/037517, International Filing Date: June 4, 2010.

1. "Methods to Identify Macromolecule Binding and Aggregation Prone Regions in Proteins and Uses Therefor,", U.S. Patent No.: 9,922,164, Date of Patent: Mar. 20, 2018, PCT/US2009/047954, International Filing Date: June 19, 2009.

Invited Talks and Plenary Lectures:

160. November 20, 2019, "Machine Learning for Developability and Formulation Design," CDD for Biologics, Boston, MA.

159. October 30, 2019, "Ethical Issues in AI and Implications for the Law," Artificial Intelligence Driving Life Sciences, Cambridge, MA.

158. October 23, 2019, "Continuous Lyophilization of Unit Doses," Lyophilization USA, Boston, MA.

157. September 26, 2019, “Continuous Manufacturing: State of the Art, Challenges, and Future Prospect,” IMA conference “Can’t Stop the Future: Spotlight on Continuous Manufacturing,” Bologna, Italy.

156. June 11, 2019, “Formulation Starts in Discovery,” Gordon Research Conference on Preclinical Form and Formulation, Waterville Valley, NH.

155. May 14, 2019, “Developability and Machine Learning for Formulation Design,” Biovia Community Day, Dusseldorf, Germany (via webcast).

154. February 27, 2019, “Living a Life of Leisure While Teaching Science in a Classical Secondary School Education,” Great Heats Academies, Sandra Day O'Connor College of Law, Phoenix, Arizona.

153. December 1, 2018, “Truths About Quantum Mechanics,” St. John’s College, Santa Fe, NM.

152. November 7, 2018, “Product and Process Development Start in Discovery,” Takeda Pharmaceutical Company, Cambridge, MA.

151. October 25, 2018, “Product and Process Development Start in Discovery,” Biovia Community Day, Boston, MA.

150. September 10, 2018, “Developability for Biologics and Approaches to Formulation Design,” BioMan Process Intensification Conference, Cambridge, MA.

149. August 3, 2018, “Biomolecular Computational Methods for Protein Engineering Against Aggregation and Other Molecular Liabilities,” Acceleron Pharma, Cambridge, MA.

148. May 30, 2018, “Continuous Lyophilization of Pharmaceutical Products in Unit Doses,” Hudson Valley LyoMac Webinair.

147. December 7, 2017, “Enabling Developability via Molecular Modeling,” CDD for Biologics, Boston, MA.

146. December 1, 2017, “The Significance of Quantum Mechanics,” St. John’s College, Annapolis, MD.

145. October 17, 2017, “Biomolecular Computational Methods for Protein Engineering Against Aggregation and Other Molecular Liabilities”, Biovia Community Day, Cambridge, MA.

144. September 21, 2017, “Developability for Biologics and Approaches to Formulation Design,” Biologics, Modeling, and Informatics (BMI) Discussion Group, Cambridge, MA.

143. July 19, 2017, “Biopharmaceuticals and Continuous Manufacturing,” Senate Competitive Caucus, U.S. Senate, Washington D.C.

142. May 10, 2017, “New Continuous Crystallization Technologies for Small Molecule Pharmaceutical Manufacturing,” Vertex Pharmaceuticals, Boston, MA.

141. April 13, 2017, “Ethics and Engineering: How to Think About the Ethics of AI,” MIT Course 6 Super UROP, Cambridge, MA.

140. February 10, 2017, “New Technologies for Holistic Pharmaceutical Creation,” United States Pharmacopeia, Rockville, MD.

139. February 1, 2017, “New Technologies for Holistic Pharmaceutical Creation: Focus on 3D Printing,” Takeda, Zurich, Switzerland.

138. January 31, 2017, “Developability and Manufacturability in Pharmaceutical Creation,” Roche, Basel, Switzerland.

137. January 31, 2017, “Developability and Manufacturability in Pharmaceutical Creation,” Lonza, Basel, Switzerland.

136. December 15, 2016, “Enabling Developability Via Molecular Modeling,” IBC Antibody Engineering & Therapeutics, San Diego, CA.

135. October 26, 2016, “Integrating Discovery, Development and Manufacturing in Pharmaceutical Creation,” University of Pennsylvania Department of Chemical and Biomolecular Engineering, Philadelphia, PA.

134. May 13, 2016, “Quantum Mechanics and Political Philosophy,” MIT Conference on Mastery of Nature, Cambridge, MA.

133. March 17, 2016, “Ethics in Engineering,” MIT Course 6 Super-UROP, Cambridge, MA.

132. October 5, 2015, “New Technologies for Enabling Continuous Manufacturing,” PQRI Meeting, Bethesda, MD (plenary lecture)

131. September 16, 2015, “Rational Approaches for the Developability of Biotherapeutics” Boston University Department of Physical Chemistry, Boston, MA

130. September 7, 2015, “MIT’s Success at Teaching and Research,” National Polytechnic University, Yerevan, Armenia

129. June 4, 2015 “Continuous Processing in (Bio)Pharmaceutical Manufacturing,” Ipsen Corporation, Paris, FR

128. May 15, 2015 "Advanced Formulation, Stabilization, and Manufacturing of Therapeutic Antibodies" MassBiologics, Boston, MA

127. April 29, 2015 "Continuous Pharmaceutical Manufacture and Advances in Biopharmaceuticals Formulation" The Pall Corporation Technology Symposium, Cambridge, MA. (Keynote Address)

126. April 14, 2015 "Rational Approaches for the Development of Biotherapeutics,"4th International Symposium on Higher Order Structure of Protein Therapeutics, Boston, MA

125. March 27, 2015 "Molecular and Macroscopic Engineering of Small Molecular Crystallization," Department of Mechanical and Chemical Engineering, ETH, Zurich, Switzerland

124. March 24, 2015 "Holistic Pharmaceutical Process Development," Department of Mechanical and Chemical Engineering, ETH, Zurich, Switzerland

123. Sept. 16, 2014 "Enabling Technologies for the Continuous Manufacturing of APIs: Continuous Crystallization" at FDA/PQRI Conference, Silver Spring, MD

122. June 10, 2014 "How 'Continuous' Manufacturing will Transform Biotherapeutic Manufacturing" The Annual Bio Manufacturing & Process Innovation Leaders Summit USA 2014 (MANU-BIO), Boston, MA (Keynote Address)

121. June 6, 2014 "Strategic Approaches for Understanding and Hindering Aggregation" IBC's Protein Aggregation, Stability & Solubility Conference, San Francisco, CA (Keynote Address)

120. March 26, 2014 "Rational Approaches to Developability and Manufacturability" Accelyrs, Cambridge, MA

119. March 21, 2014 "Rational Approaches to Developability and Manufacturability" Bayer, Wuppertal, Germany

118. January 21, 2014 "Rational Approaches for Biologics and Small Molecule Pharmaceutical Development and Manufacturing" Columbia University, New York, NY

117. January 8, 2014 "Rational Approaches to Developability and Manufacturability" Pfizer, Cambridge, MA

116. December 16, 2013 "Rational Approaches to Developability and Manufacturability"BMS, Devens, MA

115. November 7, 2013, "Recent Updates at the Novartis-MIT Center for Continuous Manufacturing", FDA, Silver Spring, MD

114. November 5, 2013 "Transforming Manufacturing to "Continuous": Flexible API and Final Dosage Form" ISPE Meeting, Washington, DC

113. October 21, 2013 "Transforming Small Molecule Pharmaceutical Manufacturing to Continuous and the Potential for Continuous Biologics Manufacturing," Integrated Continuous Biomanufacturing, an ECI Conference, Barcelona, Spain (Keynote Address)

112. September 11, 2013 "Rational Approaches to Developability and Manufacturability," Biogen Idec, Cambridge, MA

111. September 10, 2013 "Rational Approaches to Developability and Manufacturability," Pfizer, Andover, MA

110. July 10, 2013 "What Molecular Modeling in Pharmaceutical Development Can Do for You," BMS Symposium on Modeling, New Brunswick, NJ (Keynote Address)

109. June 27, 2013 "Capitalizing on Continuous Manufacturing," 8th Global Pharma Manufacturing Summit, Boston, MA (Plenary Lecture)

108. June 12, 2013, "Transforming Small Molecule Pharmaceutical Manufacturing to Continuous and the Potential for Continuous Biologics Manufacturing," Biomanufacturing Leaders Summit, Boston, MA (Keynote Address)

107. April 24, 2013 "From Molecular Computations to Continuous Manufacturing and Their Role in Shaping a Sustainable Future," 9th European Congress of Chemical Engineering, The Hague, Netherlands (Plenary Lecture)

106. April 19, 2013 "Transforming Pharmaceutical Manufacturing Continuous: The Ultra Lean Way of Manufacturing," Pharmintech, Bologna, Italy (Keynote Address)

105. March 26, 2013, "Rational Approaches to Developability for Stabilization Against Aggregation and Other Routes," 6th Annual Proteins Conference, London, UK.

104. November 15, 2012, "Rational Approaches to Developability, Formulation, and Design of Biobetters," MIT Center for Biomedical Innovation: Biomanufacturing Summit, Cambridge, MA

103. November 14, 2012, "Advanced manufacturing for pharmaceuticals and the Novartis-MIT center for continuous manufacturing," MIT ILP R&D Conference, Cambridge, MA

102. August 21, 2012, "Technical Update for the FDA on the Downstream Continuous Manufacturing Toolbox," FDA, Cambridge, MA

101. May 5, 2012, "Rational Approaches to the Stabilization of Biologics: Incorporating Developability and Manufacturability," Ispen, Milford, MA.

100. November 18, 2011, "Protein Aggregation Modeling and Novel Excipients for Downstream Processing: Incorporating Rational Approaches to Developability and Manufacturability for Biotherapeutics," BioMan, Cambridge, MA.

99. November 9, 2011, "Predication of Aggregation Prone Regions in Proteins: Incorporating Rational Approaches to Developability and Manufacturability for Biotherapeutics," CASSS Symposium on Immunogenicity, Gaithersburg, MD

98. October 20, 2011, "Heterogeneous Crystallization of API's on Excipients for "Continuous" Process and Product Design," Peck Symposium at Purdue University, West Lafayette, IN

97. October 19, 2011, "Transforming Pharmaceutical Development and Manufacturing with Molecular Computations ," AIChE Annual Symposium, CoMSEF Award, Minneapolis, MN

96. September 15, 2011, "Transforming Pharmaceutical Manufacturing, Continuous: The Ultra Lean Way of Manufacturing," President Obama's Advanced Manufacturing Partnership, Cambridge, MA

95. August 4, 2011 "Rational Approaches to Stabilization: Incorporating Developability in Discovery through Development Phases," GSK, King of Prussia, PA

94. July 28, 2011 "Rational Approaches to Stabilization: Incorporating Developability in Discovery through Development Phases," Pfizer Research, Cambridge, MA

93. July 21, 2011, "Molecular Modeling Approaches for Predicting The Stability of Biotherapeutics, Antibodies in Particular," Colorado Protein Stability Conference , Breckenridge, CO

92. May 19, 2011, "Computational Approaches for Identifying Degradation "Hotspots": Spatial Aggregation Propensity and Implementation in Pipeline Pilot,"Accelrys North America-UGM Conference, Newark, NJ

91. March 29, 2011, "Modeling Protein Degradation Processes and the Development of Rational Approaches to Stabilization," ACS, Anaheim, CA (Plenary Lecture)

90. March 15, 2011, "Transforming Pharmaceutical Manufacturing Continuous: The Ultra Lean Way of Manufacturing," ISPE-NJ

89. November, 2010, "Modeling Protein Degradation Processes and the Development of Rational Approaches to Stabilization and Protein-Cosolute Interactions: A New Strategy of Molecular QbD," AAPS Annual Meeting, New Orleans, LA

88. October, 2010, "Modeling Protein Degradation Processes and the Development of Rational Approaches to Stabilization and Protein-Cosolute Interactions: A New Strategy of Molecular QbD," PEGS Biotechnology conference, Hannover, Germany

87. September, 2010, "Modeling Protein Degradation Processes and the Development of Rational Approaches to Stabilization and Protein-Cosolute Interactions: A New Strategy of Molecular QbD," Ipsen Corporation, Milford, MA

86. September, 2010, "Modeling Protein Degradation Processes and the Development of Rational Approaches to Stabilization and Protein-Cosolute Interactions: A New Strategy of Molecular QbD," IBC Protein Formulation Conference, Providence, RI

85. August, 2010, "Molecular Modeling for the Rational Control of Polymorphism and Morphology," Sepracor Corporation, Marlborough, MA

84. July, 2010, "Modeling Protein Degradation Processes and the Development of Rational Approaches to Stabilization and Protein-Cosolute Interactions: A New Strategy of Molecular QbD," MedImmune Corporation, Gaithersburg, MD

83. July, 2010, "Continuous Manufacturing: The Ultimate in Quality by Design," Sepracor Corporation, Marlborough, MA

82. May, 2010, "Modeling Protein Degradation Processes and the Development of Rational Approaches to Stabilization and Protein-Cosolute Interactions: A New Strategy of Molecular QbD," Accelrys Annual International Conference, Boston, MA

81. April, 2010, "Modeling Protein Degradation Processes and the Development of Rational Approaches to Stabilization and Protein-Cosolute Interactions: A New Strategy of Molecular QbD," ISPE Biotech Meeting, Cambridge, MA

80. April, 2010, "Modeling Protein Degradation Processes and the Development of Rational Approaches to Stabilization and Protein-Cosolute Interactions: A New Strategy of Molecular QbD," Merck, West Point, PA

79. March, 2010, "Modeling Protein Degradation Processes and the Development of Rational Approaches to Stabilization and Protein-Cosolute Interactions: A New Strategy of Molecular QbD," Genzyme, MA

78. March, 2010, "Molecular Modeling for the Rational Control of Polymorphism and Morphology," Gilead Corporation, Foster City, CA

77. March, 2010, "Modeling Protein Degradation Processes and the Development of Rational Approaches to Stabilization and Protein-Cosolute Interactions: A New Strategy of Molecular QbD," Genentech, South San Francisco, CA

76. March, 2010, "Modeling Protein Degradation Processes and the Development of Rational Approaches to Stabilization and Protein-Cosolute Interactions: A New Strategy of Molecular QbD," Amgen, Thousand Oaks, CA

75. March, 2010, "Modeling Protein Degradation Processes and the Development of Rational Approaches to Stabilization and Protein-Cosolute Interactions: A New Strategy of Molecular QbD," Biogen-Idec, Cambridge, MA

74. December, 2009, "Continuous Manufacturing of Small Molecule Pharmaceuticals," Leaders for Global Manufacturing, MIT, Cambridge, MA

73. November, 2009, "Order parameter methods for reactions in complex systems," Princeton Center for Theoretical Sciences, Department of Physics, Princeton, NJ

72. October, 2009, "Rational approaches to protein and antibody stabilization," Schering-Plough, Elizabeth, NJ

71. September, 2009, "Rational approaches to protein and antibody stabilization," Merck & Co., West Point, PA.

70. September, 2009, "Modeling of crystallization processes," Merck Research Laboratories, Rahway, NJ.

69. September, 2009, "Rational approaches to pharmaceutical manufacturing," Merck Research Laboratories, Rahway, NJ.

68. July, 2009, "Continuous manufacturing: the ultra lean way of manufacturing," Biochemical Engineering XVI, Burlington, VT.

67. June, 2009, "Rational approaches to protein and antibody stabilization," Bristol-Meyers Squibb, New Brunswick, NJ.

66. April, 2009, "Reactivity in complex systems," University of Washington.

65. March, 2009, "Reactivity in complex systems," North Carolina Theory Seminar.

64. February, 2009, "Reactivity in complex systems," UCLA.

63. September, 2008, "Continuous manufacturing of pharmaceuticals: the ultra lean way of manufacturing," Global Pharmaceutical Manufacturing Summit, Chicago.

62. June, 2008, "Rational design of solvent formulations via molecular computations," American Association of Pharmaceutical Science National Biotechnology Conference, Toronto, Canada.

61. March, 2008, “Frontiers in chemical reactivity and pharmaceutical manufacturing,” Department of Chemical Engineering, University of Puerto-Rico.

60. March, 2008, “Frontiers in chemical reactivity and pharmaceutical manufacturing,” Department of Chemical and Biomolecular Engineering, University of Illinois, Urbana-Champaign.

59. Oct., 2007, “Formulation approaches for the future,” IBC Life Sciences on Formulation Strategies for Protein Therapeutics, Hynes Convention Center, Boston, Keynote Address.

58. July, 2007, “Understanding reaction processes in complex media such as liquids,” Gordon Conference on the Chemistry of Liquids, Holderness School, New Hampshire

57. June, 2007, “Molecular Design of New Excipients for Large Molecule Stabilization,” AAP National Biotechnology Conference, San Diego, CA.

56. March, 2007, “Finding reactions coordinates for complex processes via likelihood maximization,” ACS Spring Meeting, Chicago, IL.

55. November, 2006, “Understanding complex reaction processes,” Department of Chemical Engineering, University of Buffalo, Buffalo, New York.

54. July, 2006, "Molecular simulations of ice and gas hydrate nucleation," Physics and Chemistry of Ice Conference, Bremerhaven, Germany, Keynote Address.

53. June, 2006, “Reaction coordinates from likelihood maximization,” U.S.-Poland Workshop on Nanoscience and Nanostructured Materials, Poznan, Poland.

52. June, 2006, “Understanding complex reaction processes with applications to pharmaceuticals and heterogeneous catalysis,” Department of Chemistry, University of Western Ontario, London, Ontario, Canada.

51. February, 2006, “Statistical physics applied to the development of biopharmaceuticals,” Department of Physics, University of Rome “La Sapienza,” Rome, Italy.

50. February, 2006, “Statistical physics applied to the development of biopharmaceuticals,” SISSA, International School for Advanced Studies, Trieste, Italy.

49. September, 2005, “Molecular engineering of chemical systems,” Department of Chemical Engineering, Drexel University, Philadelphia, Pennsylvania.

48. September, 2005, “Molecular engineering of chemical systems,” Department of Chemical Engineering, Texas A&M, College Station, Texas.

47. September, 2005, "Reactivity in complex systems," Meeting in honor of Michele Parrinello's 60th Birthday, Agno, Switzerland.

46. July, 2005, "Molecular computational engineering: mechanism of methionine oxidation and rational design of additives for hindering aggregation," Protein Stability Conference, Breckenridge, Colorado.

45. May, 2005, “Transition Path Sampling Calculations in Complex Systems or How Can We Find the Reaction Coordinate?” 2005 International Conference on Scientific Computation and Differential Equations (SciCADE), Nagoya, Japan.

44. March, 2005, "Molecular computations for predictions of clathrate-hydrate nucleation and phase-behavior of multi-component hydrates," Hydrate Symposium at the American Chemical Society Spring Meeting, San Diego, California.

43. March, 2005, "Water structuring in phase transitions and in chemical reactions at sulfur sites in proteins," Water: Structure, Dynamics and Reactions Across the Phase Diagram at the American Chemical Society Spring Meeting, San Diego, California.

42. July, 2004, "A unified approach for the nucleation of ice and ice-like systems in homogeneous and inhomogeneous environments," Telluride Workshop on Studies of ice, icy particles, ice surfaces, and ice-adsorbate interactions: a molecular view," Telluride, Colorado.

41. April, 2004, "Molecular analyses and design for the stabilization of therapeutic proteins," Department of Chemical Engineering, Tufts University, Medford, Massachusetts.

40. April 2004, "Molecular analyses and design for the stabilization of therapeutic proteins," Department of Chemistry, Boston University, Boston, Massachusetts.

39. March, 2004, "Molecular analyses and design for the stabilization of therapeutic proteins," Department of Chemical Engineering, Cornell University, Ithaca, New York.

38. March, 2004, "Reactivity for phase transitions, zeolites, and biological systems," Department of Chemical Engineering, University of Rochester, Rochester, New York.

37. February, 2004, "Molecular analyses and design for the stabilization of therapeutic proteins," Department of Chemical Engineering, Tsinghua University, Beijing, China.

36. February, 2004, "Reactivity for phase transitions, zeolites, and biological systems," Department of Chemistry, Fudan University, Shanghai, China.

35. February, 2004, "Reactivity for phase transitions, zeolites, and biological systems," Center for Atomic-Scale Materials Physics (CAMP) and Department of Physics, Technical University of Copenhagen, Copenhagen, Denmark.

34. November, 2003, "Ordering of water in phase transitions and biological systems," Department of Chemistry, Washington University, St. Louis, MO.

33. November, 2003, "Ordering of water in phase transitions and biological systems," Department of Physics, University of Missouri, Columbus, MO.

32. October, 2003, "Nucleation and growth of clathrate-hydrates and ice and a new theoretical framework to address those," Dartmouth University, Thayer School of Engineering, Dartmouth, NH.

31. September, 2003, "Finding reaction pathways for industrial chemical problems," Statistical Mechanics of Rare Events, Paris, France.

30. September, 2003, "Analyses of reactions in acid zeolites and of proteins via nudged elastic band calculations and Car-Parrinello simulations," CECAM Workshop on Reactivity, Lyon, France.

29. May, 2003, "Reactivity of acidic zeolites via quantum chemical and Car-Parrinello molecular dynamical methods," Advances in the Understanding and Application of Catalysis, Moscow, Russia, *Plenary Lecture*.

28. April, 2003, “Solvation effects in clathrate-hydrates and biological systems,” Department of Chemical Engineering, Princeton University, Princeton, NJ.

27. April, 2003, “Solvation effects in clathrate-hydrates and biological systems,” Department of Chemical Engineering, University of Pittsburgh, Pittsburgh, PA.

26. March, 2003, “Solvation effects in clathrate-hydrates and biological systems,” Department of Chemical Engineering, University of Texas, Austin, TX.

25. March, 2003, "Reactivity of acidic zeolites via quantum chemical and Car-Parrinello molecular dynamical methods," invited talk in “Mechanistic Surface Chemistry,” Spring Meeting of the American Chemical Society, New Orleans, LA.

24. March, 2003, "Effects of solvation on biological processes," invited talk in “Symposium in Honor of Professor Clayton J. Radke, recipient of the American Chemical Society Award in Colloid Chemistry,” Spring Meeting of the American Chemical Society, New Orleans, LA.

23. March, 2003, February, 2003, “Solvation effects in clathrate-hydrates and biological systems,” Department of Chemical Engineering, Stanford University, Palo Alto, CA.

22. February, 2003, “Solvation effects in clathrate-hydrates and biological systems,” Department of Chemical Engineering, Tsinghua Univeristy, Beijing, China.

21. February, 2003, “Solvation effects in clathrate-hydrates and biological systems,” Department of Chemical Engineering, North Carolina State University, Raleigh, NC.

20. November, 2002, “Solvation effects in clathrate-hydrates and biological systems,” Department of Chemical Engineering, University of California, Berkeley, CA.

19. November, 2002, “Solvation effects in clathrate-hydrates and biological systems,” Department of Chemical Engineering, California Institute of Technology, Pasadena, CA.

18. July, 2002, “Nucleation of and transport in clathrate-hydrates and ice,” Physics and Chemistry of Ice Conference, New Foundland, Canada.

17. June 2002, “Quantum mechanical calculations applied to engineering problems,” Steacie Institute of Molecular Sciences, National Research Council, Ottawa, Ontario, Canada.

16. April, 2002, “Molecular simulations for the stabilization of therapeutic proteins and the quantification of nucleation of clathrate-hydrates,” Rensselaer Polytechnic Institute, Troy, NY.

15. April, 2002, “Quantification of reactive sites in zeolitic and transition metal catalysts via first-principles,” ACS Meeting, Orlando, Fl.

14. February, 2002, “The identification and study of sites of varying activity in zeolites and transition metal catalysts,” First-Principles Catalysis, Vienna, Austria.

13. February, 2002, “Order-disorder transitions on the surface of ice and in bulk ice and clathrate-hydrates,” Swiss Center for Computational Sciences, Manno, Switzerland.

12. February, 2002, “Molecular simulations for the stabilization of therapeutic proteins and the quantification of nucleation of clathrate-hydrates,” Colorado School of Mines, Golden, CO.

11. August, 2001, “Car-Parrinello simulations of the disordering of ice and dissociation of HCl, relevant to stratospheric chemistry,” ACS Meeting, Chicago, IL.

10. July, 2001, “Insight into the stabilization of therapeutic proteins via molecular simulations,” National University of Singapore, Singapore.

8. June, 2001, “Insight into the stabilization of therapeutic proteins via molecular simulations,” Hong Kong University of Science and Technology, Hong Kong.

8. April, 2001, “Multi-scale modeling of hydrate-clathrates from first-principles to macroscopic thermodynamics,” University of Connecticut, Storrs, CT.

6. February, 2001, “Multi-scale modeling of hydrate-clathrates from first-principles to macroscopic thermodynamics,” Georgia Institute of Technology, Atlanta, GA.

6. January, 2001, “Multi-scale modeling of hydrate-clathrates from first-principles to macroscopic thermodynamics,” National University of Singapore, Singapore.

5. November 1999, “Sustainable development,” ΤΒΠ Leonardo Lecture, MIT.

4. June, 1999, “Application of molecular modeling to automotive catalysis,” Workshop held at Ford Motor Company, Dearborn.

3. March, 1999, “Defect structure and its relation to methanol activation”, ACS Annual Conference, Annaheim, CA.

2. April, 1998, “Quantum mechanical methods in catalysis: a primer”, New England Catalysis Society, Worchester, MA.

1. September, 1996, “Dynamic Monte Carlo study of reaction and diffusion sites in ZSM-5 Zeolites”, Technical University of Athens, Athens, Greece.

Professional Affiliations:

AIChE, ACS, ASEE, AAPS

Languages:

French, German, Ancient Greek