

# Qiang (David) Wang

Associate Professor

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## RESEARCH INTERESTS

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- Systems:** Soft Materials, Block Copolymers, Polymer Brushes, Polyelectrolytes, Polymer Blends, Nanocomposites.
- Subjects:** Fluctuation/Correlation Effects, Self- and Directed Assembly, Surface and Interface Phenomena, Structure-Property Relations.
- Methods:** Molecular Simulations, Field Theories, Integral-Equation Theories, Density-Functional Theories, Mesoscopic Simulations, Systematic Coarse-Graining, Statistical Mechanics.

## PROFESSIONAL PREPARATION

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B. E.	Chemical Engineering	Tsinghua University, Beijing, P. R. China	1993
Ph. D.	Chemical Engineering	University of Wisconsin – Madison <i>Advisors: Prof. Juan de Pablo &amp; Prof. Paul Nealey</i>	2002
Postdoctoral Researcher	Chemical Engineering Materials Research Lab.	University of California – Santa Barbara <i>Advisor: Prof. Glenn Fredrickson</i>	2002-2004

## APPOINTMENTS

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Assistant Professor	Dept. of Chem. & Biol. Eng.	Colorado State University	2004-2010
Assistant Professor	School of Biomed. Eng.	Colorado State University	2007-2010
Associate Professor	Dept. of Chem. & Biol. Eng. and School of Biomed. Eng.	Colorado State University	2010-
Visiting Professor	Polymer Theory Group <i>Host: Prof. Dr. Kurt Kremer</i>	Max Planck Institute for Polymer Research, Mainz, Germany	1-8/2013

## SELECTED HONORS AND AWARDS

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- George T. Abell Outstanding Early-Career Faculty Award, College of Engineering, CSU, 2009.
- Faculty Early Career Development (CAREER) Award, National Science Foundation, 2008.
- Nominee for the Outstanding Honors Academic Adviser Award, CSU, 2008.
- The Petroleum Research Fund Type G Award, American Chemical Society, 2007.

## STUDENTS AND POSTDOCTORAL RESEARCHERS SUPERVISED

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- 5 Postdoctoral researchers: *Vijay Gupta (2013-), Pengfei Zhang (2011-), Xinghua Zhang (2009-10), Yuhua Yin (2007-08), Ying Jiang (2006-07).*
- 5 PhD students: *Yawei Li (2013-), Ms. Jacqueline Acres (2010-11), Delian Yang (2009-), Jing Zong (2008-), Dong Meng (2004-09).*
- 2 MS students: *Paramvir Sandhu (2011-12), Lawrence Kaneria (2007-08).*
- 5 Undergraduate students: *William Masters, Christopher Driscoll, Brian Miller, Ms. Jacqueline Acres, Gabor Mate.*

## COURSES TAUGHT

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- Thermodynamic Process Analysis (undergraduate course), Spring 2006~2012 (except 2008), CSU.
- Advanced Computational Methods for Materials (graduate course), Spring 2008, CSU.
- Chemical Engineering Thermodynamics (graduate course), Fall 2004~2012, CSU.

## SYNERGISTIC ACTIVITIES

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- **Member** of the *American Physical Society* (Division of Polymer Physics), *American Institute of Chemical Engineers*, *Materials Research Society*, and *American Chemical Society* (Division of Polymeric Materials: Science & Engineering).
- **Organizer** of the Focus Session “*Understanding Fluctuation and Correlation Effects in Polymers?*” at APS March meeting 2013; **Co-organizer** of NSF Workshop on *Mathematical Modeling and Computer Simulations for Soft Materials*, CSU, September 13-17, 2010; **Panelist** of NSF Workshop on *Molecular Models for Carbon-Neutral Industrialization*, Palm Desert, CA, April 9-10, 2010; **Session chair** for “*Dynamics of Polymers on Multi-Length Scales: Solutions?*” at APS March meeting 2010; **Session co-chair** for “*Polymer Thin Films and Interfaces P?*” at AIChE 2007 Annual Meeting.
- **Reviewer** of more than 70 manuscripts for 14 academic journals (*ACS Macro Lett.*, *ACS Nano*, *Commun. Comput. Phys.*, *Eur. Phys. J. E*, *J. Chem. Phys.*, *J. Phys. Chem. B*, *J. Polym. Sci. Part B: Polym. Phys.*, *Langmuir*, *Macromol. Theory Simul.*, *Macromolecules*, *Phys. Chem. Chem. Phys.*, *Phys. Rev. E*, *Phys. Rev. Lett.*, and *Soft Matter*); **Panel and ad hoc reviewer** of research proposals for DOE, NSF, ACS-PRF, and SHARCNET (Shared Hierarchical Academic Research Computing Network, Ontario, Canada).
- **Attendee** of NSF workshop on *Enhancement of Chemical Engineering Curricula with Biological Applications in Thermodynamics*, San Jose, CA, 2010; **Attendee** of *American Society for Engineering Education (ASEE) 14<sup>th</sup> Summer School for Chemical Engineering Faculty*, Pullman, WA, 2007.
- **Member** of the *College of Engineering Technology Committee* (Fall 2004 – Spring 2007), *Engineering Student Technology Committee* (Fall 2004 – Spring 2008), *Faculty Council Committee on Libraries* (Fall 2010 – Fall 2012), and *Department of Chemical and Biological Engineering Graduate Affairs Committee* (Spring 2012 – Fall 2012) at CSU.
- **Graduate thesis committee member** for 11 students at CSU: *Soheil Boddobi* (PhD student in Dept. of Chem. & Biol. Eng.), *Ramon Saavedra* (MS student in Dept. of Chem. Eng.), *Benjamin Kronholm*, *Ms. Isil Kayiran*, *Ercan Bayram*, *Michael Wells*, *Garret Miyake*, *Long San*, *Meghan Schmitt* (PhD students in Dept. of Chemistry), *Yang Zou*, and *Ms. Jennifer Maple* (PhD student in Dept. of Mathematics).
- **Academic advising** of 8~20 undergraduate students each semester at CSU.

## CONTRACTS AND GRANTS

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1. “*Directed Assembly of Rod-Coil Block Copolymers by Combined External Fields?*”, **DOE-BES**, \$450,000, August 15, 2011 – August 14, 2014 (PI).
2. “*CAREER: Towards Rational Design of ‘Smart’ Surfaces from Two-Component Polymer Brushes?*”, **NSF-ENG**, \$403,626, February 1, 2009 – January 31, 2014 (PI).
3. “*Workshop on Mathematical Modeling and Computer Simulations for Soft Materials?*”, **NSF-DMS**, \$24,281, June 15, 2009 – May 31, 2010 (Co-PI).
4. “*Magnetic Field Directed Self-Assembly of Conjugated Rod-Coil Block Copolymers?*”, **NSF-ENG**, \$190,000, September 1, 2007 – August 31, 2010 (Co-PI).
5. “*Achieving Three-Dimensional Well-Ordered Nanostructures in Block Copolymer Films by Combined External Fields?*”, **DOE-BES**, \$451,458, August 15, 2007 – August 14, 2011 (PI).
6. “*Modeling Polyelectrolyte Layer-by-Layer Assembly?*”, **ACS-PRF**, \$40,000, July 1, 2007 – August 31, 2009 (PI).

## PATENTS

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US Patent 6,746,825: “*Guided Self-Assembly of Block Copolymer Films on Interferometrically Nanopatterned Substrates*”, with P. F. Nealey, J. J. de Pablo, F. Cerrina, H. H. Solak, X. M. Yang, and R. D. Peters.

## BOOK CHAPTERS

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1. Q. Wang, “*Lattice/Off-Lattice Simulation of Block Copolymers*”, in **Encyclopedia of Polymeric Nanomaterials**, ed. S. Kobayashi and K. Müllen, Springer, in press.
2. Q. Wang, “*Monte Carlo Simulations of Nano-Confined Block Copolymers*”, Chap. 16 in **Nanostructured Soft Matter: Experiment, Theory, Simulation and Perspectives**, 495-527, ed. A. V. Zvelindovsky, Springer, 2007.

## PAPERS IN PEER-REVIEWED JOURNALS (*34 published, cited 839 times*)

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### From independent work at CSU:

1. D. Yang and Q. Wang, “*Systematic and Simulation-Free Coarse-Graining of Homopolymer Melts*”, **Macromolecules**, to be submitted.
2. D. Yang, J. Zong, and Q. Wang, “*Fluctuations/Correlations in Symmetric Diblock Copolymers. II. On the Disordered Phase*”, **Macromolecules**, submitted.
3. P. Zhang and Q. Wang, “*Quantitative Study of Fluctuation Effects by Fast Lattice Monte Carlo Simulations. IV. Compression of Grafted Homopolymers in an Explicit Solvent*”, **Macromolecules**, submitted.
4. D. Yang and Q. Wang, “*Structural and Phase Transitions of One and Two Polymer Mushrooms in a Poor Solvent*”, **J. Chem. Phys.**, submitted.
5. J. Zong and Q. Wang, “*Fluctuations/Correlations in Symmetric Diblock Copolymers. I. On the Order-Disorder Transition*”, **J. Chem. Phys.**, submitted.
6. P. Zhang and Q. Wang, “*Solvent Entropy and Coarse-Graining of Polymer Lattice Models*”, **Macromolecules**, submitted.
7. P. Sandhu, J. Zong, D. Yang, and Q. Wang, “*On the Comparisons Between Dissipative Particle Dynamics Simulations and Self-Consistent Field Calculations of Diblock Copolymer Microphase Separation*”, **J. Chem. Phys.** **138**, 194904 (2013).
8. J. Zong, X. Zhang, and Q. Wang, “*Fast Off-Lattice Monte Carlo Simulations of Soft-Core Spherocylinders: Isotropic-Nematic Transition and Comparisons with Virial Expansion*”, **J. Chem. Phys.** **137**, 134904 (2012). *Cited 1 times.*
9. P. Zhang, B. Li, and Q. Wang, “*Quantitative Study of Fluctuation Effects by Fast Lattice Monte Carlo Simulations. III. Homopolymer Brushes in an Explicit Solvent*”, **Macromolecules** **45** (5), 2537-2550 (2012). *Cited 2 times.*
10. D. Meng and Q. Wang, “*Stimuli-Response of Charged Diblock Copolymer Brushes*”, **J. Chem. Phys.** **135**, 224904 (2011); *selected in Vir. J. Bio. Phys. Res.* **22** (12), (2011).
11. Z. Wang, B. Li, D. Ding, and Q. Wang, “*Charge Inversion by Flexible Polyelectrolytes on Spherical Surfaces: Numerical Self-Consistent Field Calculations under the Ground-State Dominance Approximation*”, **Macromolecules** **44** (21), 8607-8613 (2011). *Cited 2 times.*
12. P. Zhang, B. Li, and Q. Wang, “*Quantitative Study of Fluctuation Effects by Fast Lattice Monte Carlo Simulations. 2. Homopolymer Brushes in an Implicit, Good Solvent*”, **Macromolecules** **44** (19), 7837-7852 (2011). *Cited 3 times.*

13. P. Zhang, X. Zhang, B. Li, and Q. Wang, “Quantitative Study of Fluctuation Effects by Fast Lattice Monte Carlo Simulations. I. Compressible Homopolymer Melts”, **Soft Matter** **7** (9), 4461-4471 (2011). Cited **3** times.
14. Q. Wang, “Theory and Simulation of Self-Assembly of Rod-Coil Block Copolymer Melts: Recent Progress”, **Soft Matter** **7** (8), 3711-3716 (2011). Cited **7** times.
15. G. Yang, P. Tang, Y. Yang, and Q. Wang, “Self-Assembled Microstructures of Confined Rod-Coil Diblock Copolymers by Self-Consistent Field Theory”, **J. Phys. Chem. B** **114** (46), 14897-14906 (2010). Cited **8** times.
16. D. Meng and Q. Wang, “Complex Morphologies in Thin Films of Symmetric Diblock Copolymers as Stable and Unstable Phases”, **Soft Matter** **6** (23), 5891-5906 (2010). **Inside Front Cover**. Cited **1** times.
17. S.-M. Park, D. Meng, C. T. Rettner, D. S. Dandy, Q. Wang, and H.-C. Kim, “Bending of Lamellar Microdomains of Block Copolymers on Non-Selective Surfaces”, **Macromolecules** **43** (3), 1665-1670 (2010).
18. Q. Wang, “On the Anisotropy of Lattice Polymers”, **J. Chem. Phys.** **131**, 234903 (2009). Cited **1** times.
19. B. Akgun, G. Ugur, W. J. Brittain, C. F. Majkrzak, X. Li, J. Wang, H. Li, D. T. Wu, Q. Wang, M. D. Foster, “Internal Structure of Ultrathin Diblock Copolymer Brushes”, **Macromolecules** **42** (21), 8411-8422 (2009). Cited **6** times.
20. Q. Wang, “Studying Soft Matter with ‘Soft’ Potentials: Fast Lattice Monte Carlo Simulations and Corresponding Lattice Self-Consistent Field Calculations”, **Soft Matter** **5** (22), 4564-4567 (2009); **6** (24), 6206-6207 (2010). Cited **7** times.
21. D. Meng and Q. Wang, “Solvent-Response of Diblock Copolymer Brushes”, **J. Chem. Phys.** **130**, 134904 (2009). Cited **11** times.
22. Q. Wang and Y. Yin, “Fast Off-Lattice Monte Carlo Simulations with ‘Soft’ Repulsive Potentials”, **J. Chem. Phys.** **130**, 104903 (2009). Cited **17** times.
23. Q. Wang, “Internal Structure and Charge Compensation of Polyelectrolyte Multilayers: A Numerical Study”, **Soft Matter** **5** (2), 413-424 (2009). Cited **7** times.
24. Q. Wang, “Effects of Interaction Range and Compressibility on Microphase Separation of Diblock Copolymers: Mean-Field Analysis”, **J. Chem. Phys.** **129**, 054904 (2008). Cited **11** times.
25. S. O. Kim, B. H. Kim, D. Meng, D. O. Shin, C. M. Koo, H. H. Solak, and Q. Wang, “Novel Complex Nanostructure from Directed Assembly of Block Copolymers on Incommensurate Surface Pattern”, **Adv. Mater.** **19** (20), 3271-3275 (2007); **20** (5), 866 (2008). **Frontispiece**. Cited **39** times.
26. D. Meng and Q. Wang, “Hard-Surface Effects in Polymer Self-Consistent Field Calculations”, **J. Chem. Phys.** **126**, 234902 (2007). Cited **24** times.
27. Q. Wang, “Symmetric Diblock Copolymers in Nanopores: Monte Carlo Simulations and Strong-Stretching Theory”, **J. Chem. Phys.** **126**, 024903 (2007). Cited **33** times.
28. M. D. Petters, S. M. Kreidenweis, J. R. Snider, K. A. Koehler, Q. Wang, A. J. Prenni, and P. J. Demott, “Cloud Droplet Activation of Polymerized Organic Aerosol”, **Tellus B** **58** (3), 196-205 (2006). Cited **10** times.
29. Q. Wang, “Modelling Layer-by-Layer Assembly of Flexible Polyelectrolytes”, **J. Phys. Chem. B** **110** (12), 5825-5828 (2006). Cited **17** times.
30. Q. Wang, “Charge Inversion by Flexible Polyelectrolytes on Flat Surfaces from Self-Consistent Field Calculations”, **Macromolecules** **38** (21), 8911-8922 (2005). Cited **28** times.

#### **From PhD and postdoctoral work:**

31. Q. Wang, “Morphology of Symmetric Diblock Copolymers Confined Between Two Stripe-Patterned Surfaces – Tilted Lamellae and More”, **Macromol. Theory Simul.** **14** (2), 96-108 (2005). **Front Cover**. Cited **16** times.
32. Q. Wang, T. Taniguchi, and G. H. Fredrickson, “Self-Consistent Field Theory of Polyelectrolyte Systems”, **J. Phys. Chem. B** **108** (21), 6733-6744 (2004); **109** (19), 9855-9856 (2005). Cited **51** times.

33. Q. Wang, P. F. Nealey, and J. J. de Pablo, “Behavior of Single Nano-Particle / Homopolymer Chain in Ordered Structures of Diblock Copolymers”, **J. Chem. Phys.** **118** (24), 11278-11285 (2003). Cited **39** times.
34. Q. Wang, P. F. Nealey, and J. J. de Pablo, “Simulations of the Morphology of Cylinder-Forming Asymmetric Diblock Copolymer Thin Films on Nano-Patterned Substrates”, **Macromolecules** **36** (5), 1731-1740 (2003). Cited **45** times.
35. Q. Wang, P. F. Nealey, and J. J. de Pablo, “Lamellar Structures of Symmetric Diblock Copolymers – Comparisons Between Lattice Monte Carlo Simulations and Self-Consistent Mean-Field Calculations”, **Macromolecules** **35** (25), 9563-9573 (2002). Cited **30** times.
36. Q. Wang, P. F. Nealey, and J. J. de Pablo, “Monte Carlo Simulations of Asymmetric Diblock Copolymer Thin Films Confined Between Two Homogeneous Surfaces”, **Macromolecules** **34** (10), 3458-3470 (2001). Cited **131** times.
37. R. D. Peters, X. M. Yang, Q. Wang, J. J. de Pablo, and P. F. Nealey, “Combining Advanced Lithographic Techniques and Self-Assembly of Thin Films of Diblock Copolymers to Produce Templates for Nanofabrication”, **J. Vac. Sci. Technol. B** **18** (6), 3530-3534 (2000). Cited **54** times.
38. Q. Wang, S. K. Nath, M. D. Graham, P. F. Nealey, and J. J. de Pablo, “Symmetric Diblock Copolymer Thin Films Confined Between Homogeneous and Patterned Surfaces: Simulations and Theory”, **J. Chem. Phys.** **112** (22), 9996-10010 (2000). Cited **69** times.
39. Q. Wang, Q. Yan, P. F. Nealey, and J. J. de Pablo, “Monte Carlo Simulations of Diblock Copolymer Thin Films Confined Between Chemically Heterogeneous Hard Surfaces”, **Macromolecules** **33** (12), 4512-4525 (2000). Cited **49** times.
40. Q. Wang, Q. Yan, P. F. Nealey, and J. J. de Pablo, “Monte Carlo Simulations of Diblock Copolymer Thin Films Confined Between Two Homogeneous Surfaces”, **J. Chem. Phys.** **112** (1), 450-464 (2000). Cited **117** times.

## INVITED TALKS, SEMINARS, AND LECTURES

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1. “Fluctuations/Correlations in Diblock Copolymer Melts: Simulations and Theories”, **Seminar**, Institute for Theoretical Physics, University of Göttingen, Göttingen, Germany, April 17, 2013.
2. “Fast Monte Carlo Simulations: Combining Particles with Fields”, **Invited Talk**, American Chemical Society (ACS) 244<sup>th</sup> National Meeting, Philadelphia, PA, August 23, 2012.
3. “Fast Monte Carlo Simulations: Combining and Comparing Particles with Fields”, **Invited Talk**, Workshop on Bridging Scales in Computational Polymer Chemistry, Institute for Computational and Experimental Research in Mathematics, Brown University, Providence, RI, August 9, 2012.
4. “Quantifying Fluctuation/Correlation Effects in Inhomogeneous Polymers by Fast Monte Carlo Simulations”, **Invited Talk**, International Conference on the Hierarchical Structures in Complex Fluids, Kavli Institute for Theoretical Physics in China, Beijing, P. R. China, July 5, 2011.
5. “Fast Monte Carlo Simulations of Soft Materials”, **Seminar**, Department of Chemical and Environmental Engineering, University of California – Riverside, Riverside, CA, May 20, 2011.
6. “Studying Polymers with Fields”, **Seminar**, Department of Engineering Mechanics, University of Nebraska – Lincoln, Lincoln, NE, September 28, 2010.
7. “Informal Tutorial on SCFT”, **Lecture** (with Prof. Carlos Garcia-Cervera), Workshop on Poly and Polymer Electrolytes for Energy Conversion: Ab Initio, Molecular, and Continuum Models, Lorentz Center, Leiden University, The Netherlands, August 24, 2010.
8. “Numerical Modeling of Polyelectrolyte Adsorption and Layer-by-Layer Assembly”, **Invited Talk**, Workshop on Poly and Polymer Electrolytes for Energy Conversion: Ab Initio, Molecular, and Continuum Models, Lorentz Center, Leiden University, The Netherlands, August 24, 2010.

9. “*Some Applications of SCFT and Its Quantitative Test by Fast Lattice Monte Carlo Simulation*”, **Invited Talk**, Workshop on Self-Assembly of Block Copolymers: Theoretical Models and Mathematical Challenges, The Banff International Research Station, Banff, Canada, May 28, 2010.
10. “*Diblock Copolymers under Nano-Confinement*”, **Keynote Address**, ACS 238<sup>th</sup> National Meeting, Washington D. C., August 19, 2009.
11. “*Studying Polymers with Fields and Particles*”, **Seminar**, Department of Chemistry, Colorado State University, Fort Collins, CO, July 1, 2009.
12. “*Studying Polymers with Fields*”, **Seminar**, Department of Physics, Colorado State University, Fort Collins, CO, February 9, 2009.
13. “*Polymer Brushes as ‘Smart’ Surfaces*”, **Seminar**, Department of Macromolecular Science, Fudan University, Shanghai, P. R. China, January 8, 2009.
14. “*Structure and Response of ‘Smart’ Polymer Brushes*”, **Invited Talk**, ACS 236<sup>th</sup> National Meeting, Philadelphia, PA, August 18, 2008.
15. “*Some Mathematical/Numerical Problems in the Study of Inhomogeneous Polymers*”, **Seminar**, Department of Mathematics, Colorado State University, Fort Collins, CO, April 24, 2008.
16. “*Studying Polymeric Materials at Nano- to Meso-Scales with Coarse-Grained Models*”, **Invited Talk**, JNC/CSU Joint Workshop on Materials Initiatives, Colorado State University, Fort Collins, CO, April 2, 2008.
17. “*Symmetric Diblock Copolymers under Nano-Confinement*”, **Seminar**, Institute of Polymer Science, Department of Chemical Engineering, Tsinghua University, Beijing, P. R. China, December 21, 2007.
18. “*Internal Structure and Charge Compensation of Polyelectrolyte Multilayers*”, **Seminar**, Institute of Chemistry, The Chinese Academy of Sciences, Beijing, P. R. China, December 13, 2007.
19. “*Symmetric Diblock Copolymers under Nano-Confinement*”, **Invited Talk**, Workshop on Structure Formation and Evolution in Soft Matter/Complex Fluid Systems, Beijing International Center for Mathematical Research, Beijing, P. R. China, December 4, 2007.
20. “*Symmetric Diblock Copolymers under Nano-Confinement*”, **Invited Talk**, 2007 Joint ACS/AIChE Rocky Mountain Regional Meeting, Denver, CO, August 30, 2007.
21. “*Symmetric Diblock Copolymers under Nano-Confinement: Theories and Simulations*”, **Seminar**, Department of Macromolecular Science, Fudan University, Shanghai, P. R. China, June 25, 2007.
22. “*Symmetric Diblock Copolymers under Nano-Confinement: Theories and Simulations*”, **Seminar**, Department of Polymer Science and Engineering, University of Science and Technology of China, Hefei, Anhui, P. R. China, June 22, 2007.
23. “*Symmetric Diblock Copolymers under Nano-Confinement: Theories and Simulations*”, **Seminar**, College of Chemistry, Nankai University, Tianjin, P. R. China, June 15, 2007.
24. “*Understanding Monte Carlo Simulations*”, **Lecture Series**, College of Physics, Nankai University, Tianjin, P. R. China, June 4~15, 2007.
25. “*Internal Structure and Charge Compensation of Polyelectrolyte Multilayers*”, **Seminar**, Chemical Engineering Department, Colorado School of Mines, Golden, CO, February 2, 2007.
26. “*Charge Inversion and Layer-by-Layer Assembly of Flexible Polyelectrolytes on Flat Surfaces*”, **Seminar**, Department of Chemical Engineering, Colorado State University, Fort Collins, CO, April 22, 2005.

## **PLUS ~110 TALKS AND POSTERS AT PROFESSIONAL CONFERENCES**

<http://lamar.colostate.edu/~qwang/presentations.htm>