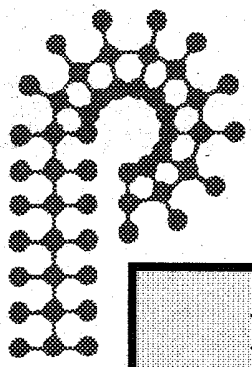

MOLECULAR SIMULATION OF STRUCTURE AND PROPERTIES IN POLYMER SYSTEMS

AN INTERDISCIPLINARY WORKSHOP

sponsored by:

the division of polymer chemistry, inc.

AMERICAN CHEMICAL SOCIETY

XEROX CORPORATION

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MOLECULAR SIMULATIONS INC.

Asilomar Conference Center
Pacific Grove, California

October 17 - 20, 1993

Molecular Simulation of Structure and Properties in Polymer Systems

WORKSHOP ORGANIZERS

Tom A. Kavassalis, *Xerox Research Centre of Canada*

Shaw-Ling Hsu, *University of Massachusetts*

SPECIAL THANKS TO . . .

Diane M. Morrill, *Business Manager, ACS Polymer Division*

Thomas W. Smith, *Workshops Chair, ACS Polymer Division*

Thomas J. Pacansky, *Treasurer, ACS Polymer Division*

Robert W. Stackman, *Assistant Treasurer, ACS Polymer Division*

Sharon Cottle and **Jennifer Dow**, *Xerox Research Centre of Canada*

SUNDAY, OCTOBER 17, 1993

4:00 p.m.	**Registration**
5:00 p.m.	**Reception**
6:00 - 7:00 p.m.	**Dinner**
7:30 p.m.	**Plenary Lecture** **Dynamics of Proteins: Temperature Echoes and Protein Folding** *speaker:* **M. Karplus**, *Harvard University*

MONDAY, OCTOBER 18, 1993

Prediction of Polymer Structure and Properties

Chair: M. Karplus

7:30 a.m.	**Breakfast**
8:45 a.m.	**Transport and Solubility of Small Molecules in Solid Polymers** *speaker:* **U. Suter**, *ETH-Zurich*
9:30 a.m.	**Molecular Simulations of Amorphous Polymers** *speaker:* **J. H. R. Clarke**, *UMIST, Manchester*
10:15 a.m.	**Break**
10:30 a.m.	**Simulation and Analysis of Chain-Molecule Transitions** *speaker:* **A. J. Hopfinger**, *University of Illinois, Chicago*
11:15 a.m.	**A Comparison of United Atom and Explicit Atom Models in Simulations of Polyethylene Melts** *speaker:* **D. Y. Yoon**, *IBM Almaden Research Center*
12:00 - 1:00 p.m.	**Lunch**
6:00 - 7:00 p.m.	**Dinner**

The Link Between Experimentation and Molecular Simulation

Chair: S. L. Hsu

7:30 p.m.	**Properties of Ensemble-Averaged Vibrational Spectra of Flexible Chain Molecules** *speaker:* **R. G. Snyder**, *University of California, Berkeley*
8:15 p.m.	**X-Ray Studies of Transesterfication in Thermotropic Copolyesters** *speaker:* **J. Blackwell**, *Case Western Reserve University*

Molecular Simulation of Structure and Properties in Polymer Systems

TUESDAY, OCTOBER 19, 1993

Molecular Simulation and Phase Behaviour
Chair: U. Suter

7:30 a.m.	**Breakfast**
8:45 a.m.	**Pattern Selection in Complex Fluids** *speaker:* **M. Muthukumar**, *University of Massachusetts*
9:30 a.m.	**Isotropic/Nematic Phase Behaviours in Rigid Rod Systems** *speaker:* **I. C. Sanchez**, *University of Texas, Austin*
10:15 a.m.	**Break**
10:30 a.m.	**Molecular Simulation of Chain Molecules and their Phase Behaviours** *speaker:* **J. de Pablo**, *University of Wisconsin*
11:15 a.m.	**Entropic Phase Transitions in Simple and Complex Fluids** *speaker:* **D. Frenkel**, *FOM, Amsterdam*
12:00 - 1:00 p.m.	**Lunch**
4:00 - 6:00 p.m.	**Poster Session**
6:00 - 7:00 p.m.	**Dinner**

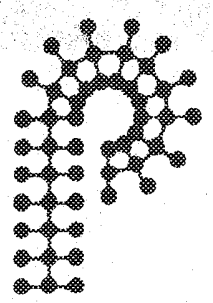
The Link Between Experimentation and Molecular Simulation
Chair: I. C. Sanchez

7:30 p.m.	**Simulations of Self-Assembled Block Copolymers** *speaker:* **W. Mattice**, *University of Akron*
8:15 p.m.	**Compositional Heterogeneity or Clustering in Hydrogen Bonded Polymer Blends** *speaker:* **P. C. Painter**, *Pennsylvania State University*

WEDNESDAY, OCTOBER 20, 1993

New Developments in Molecular Simulation
Chair: T. A. Kavassalis

7:30 a.m.	**Breakfast**
8:45 a.m.	**MD of Polymers in Solution Subject to Shear Flow** *speaker:* **J.-P. Rychaert**, *Université Libre de Bruxelles*
9:30 a.m.	**Mobility of Small Particles in Amorphous Polymers** *speaker:* **F. Müller-Plathe**, *ETH-Zurich*
10:15 a.m.	**Break**
10:30 a.m.	**Small Molecules, Big Calculations: Application of MO Methods to Polymer Mixtures** *speaker:* **C. H. Reynolds**, *Rohm and Haas Company*
11:15 a.m.	**New Developments for Million Atom Simulations** *speaker:* **W. A. Goddard, III**, *California Institute of Technology*
12:00 - 1:00 p.m.	**Lunch**



Poster Presentations

1. **"Statistical Mechanics of Liquid Crystal Flow"**
   authors: **S. Sarman** and **P. Cumming**, *Department of Chemical Engineering, University of Virginia* and **D. J. Evans**, *Research School of Chemistry, Australian National University*

2. **"Elasticity of Solid Polymers as a Result of Thermal Motions"**
   authors: **A. A. Gusev, M. M. Zehnder** and **U. Suter**, *Institut fur Polymere, ETH-Zurich*

3. **"Substituted Poly (thionylphosphazenes) Molecular Models - Study of 'Twisted' Cis-Trans Conformations using Density Functional Theory Approach"**
   authors: **A. Raja** and **J. B. Lagowski**, *Memorial University of Newfoundland*

4. **"Molecular Dynamics Simulations of Polyethylene Crystallization"**
   authors: **P. R. Sundararajan** and **T.A. Kavassalis**, *Xerox Research Centre of Canada*

5. **"Scaling Behaviour of Some Molecular Shape Descriptors of Polymer Chains and Protein Backbones"**
   author: **G. Arteca**, *Department de Chimie et Biochimie, Laurential University*

6. **"Correlation and Prediction of Phase Diagrams for Polymer Blends Using a Nonrandom Lattice-Fluid Equation of State"**
   author: **R. G. Wissinger**, *The B. F. Goodrich Company*

Poster Presentations

7. **"Discontinuous Molecular Dynamics Simulation of Hydrogen Bonding Systems"**
   authors: **J. R. Elliott, Jr., R. Natarajan**, and **J.-X. Liu**, *University of Akron*

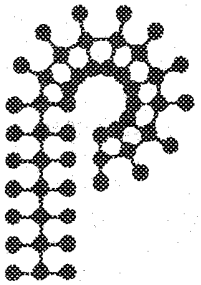
8. **"Molecular Dynamics Simulation of Vibrational Energy Transfer in a Crystalline Naphthalene"**
   authors: **H. Kim**, *Chungman National University (Korea)* and **E.-Y. Kim and Y. Won**, *Hanyang University (Korea)*

9. **"Diffusions of Small Molecules in Amorphous Nylon"**
   authors: **C. Qian, Z. M. Chen**, and **T. Cagin**, *Molecular Simulations Inc.*

10. **"Stochastic Phase Space Dynamics with Constraints and an Application to the United Atom Model for Alkanes"**
    authors: **W. Paul**, *IBM Almaden Research Center*, **G. D. Smith**, *NASA Ames Research Center*, and **D. Y. Yoon**, *IBM Almaden Research Center*

11. **"Spectral Simulation and Premelting in n-Alkanes"**
    author: **D. Cates, H. L. Strauss and R. G. Snyder**, *University of California, Berkeley*

12. **"Conformational Properties of Weakly Charged Polyelectrolytes from MC Simulations"**
    author: **C. Seidel**, *University of Minnesota*



Poster Presentations

13. **"Molecular Dynamics Simulations of Poly(oxyethylene) Melts"**
    authors: **G. D. Smith, R. L. Jaffe,** *NASA Ames Research Center,* and **D. Y. Yoon,** *IBM Almaden Research Center*

14. **"Conformational Energies of Poly(perfluoroalkanes) and Poly(perfluoroalkylethers) from Ab Initio Quantum Chemical Calculations"**
    authors: **R. L. Jaffe, G. D. Smith,** *NASA Ames Research Center* and **D. Y. Yoon,** *IBM Almaden Research Center*

15. **"Molecular Simulations of Cooperative Ring Flip Motions in Single Chains of Polystyrene"**
    authors: **R. Khare** and **M. E. Paulaitis,** *University of Delaware*

16. **"Ab Initio Models of Metal Chelation Sites in Polyimides"**
    authors: **D. D. Shillady, K. Esperdy,** and **V. Kincaid,** *Virginia Commonwealth University*

17. **"Molecular Simulation of a Nematic Liquid Crystal"**
    authors: **S. S. Patnaik, R. Pachter, R. L. Crane,** and **W. Adams,** *Materials Directorate, Wright Patterson Air Force Base*

18. **"Simulation of the Temperature Dependent Properties of the b-Phase of Crystalline Poly(vinylidene fluoride)"**
    authors: **J. Carbeck, D. J. Lacks,** and **G. C. Rutledge,** *MIT*

Poster Presentations

19. **"Geometric Characterization of Glassy Atactic Polypropylene: Prelude to a Multidimensional Transition-State Theory Description of Diffusion"**
    authors: **M. L. Greenfield** and **D. N. Theodorou**, *University of California, Berkeley*

20. **"A Connectivity-Altering Monte Carlo Scheme for the Simulation of Dense Polymer Melts"**
    authors: **P. V. K. Pant** and **D. N. Theodorou**, *University of California, Berkeley*

21. **"Computer Simulation of Polymer Adsorption Dynamics"**
    author: **J. S. Shaffer**, *University of Southern California*

22. **"Collapsed Polymer Chains and Implications on Blend Miscibility"**
    author: **G. Tanaka**, *The B. F. Goodrich Company*

23. **"Molecular Modeling of Structural Phase Transitions in Crystalline Polymers"**
    authors: **D. C. Doherty**, *Minnesota Supercomputer Center, Inc.* and **A. J. Hopfinger**, *University of Illinois, Chicago*

24. **"Tacticity Effects on Polymer Blend Miscibility"**
    author: **J. D. Honeycutt**, *BIOSYM Technologies, Inc.*

NOTES