

# Stanford

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## Hans Andersen

David Mulvane Ehram and Edward Curtis Franklin Professor in Chemistry, Emeritus

### CONTACT INFORMATION

- **Administrative Contact**

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### Bio

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### BIO

Professor Emeritus Hans C. Andersen applies statistical mechanics to develop theoretical understanding of the structure and dynamics of liquids and new computer simulation methods to aid in these studies.

He was born in 1941 in Brooklyn, New York. He studied chemistry as an undergraduate, then physical chemistry as a doctoral candidate at the Massachusetts Institute of Technology (B.S. 1962, Ph.D. 1966). At MIT he first learned about using a combination of mathematical techniques and the ideas of statistical mechanics to investigate problems of chemical and physical interest. This has been the focus of his research ever since. He joined the Stanford Department of Chemistry as Assistant Professor in 1968, and became Professor of Chemistry in 1980. He was named David Mulvane Ehram and Edward Curtis Franklin Professor in Chemistry in 1994. Professor Andersen served as department chairman from 2002 through 2005. Among many honors, his work has been recognized in the Theoretical Chemistry Award and Hildebrand Award in Theoretical and Experimental Chemistry of Liquids from the American Chemical Society, as well as the Dean's Award for Distinguished Teaching and Walter J. Gores Award for Excellence in Teaching at Stanford. He has been elected a member of the National Academy of Sciences, and a fellow of both the American Academy of Arts and Sciences and American Association for the Advancement of Science.

Professor Andersen's research program has used both traditional statistical mechanical theory and molecular dynamics computer simulation. Early in his career, he was one of the developers of what has come to be known as the Weeks-Chandler-Andersen theory of liquids, which is a way of understanding the structure, thermodynamics, and dynamics of simple dense liquids. Later, he developed several new simulation techniques – now in common use – for exploring the behavior of liquids, such as simulation of a system under constant pressure and/or temperature. He used computer simulations of normal and supercooled liquids to study the temperature dependence of molecular motion in liquids, crystallization in supercooled liquids, and the structure of amorphous solids.

Professor Andersen also developed and analyzed a class of simple lattice models, called facilitated kinetic Ising models, which were then widely used by others to provide insight into the dynamics of real liquids. He simulated simple models of rigid rod polymers to understand the dynamics of this type of material. More recently, in collaboration with Professor Greg Voth of the University of Chicago, he has applied statistical mechanical ideas to the development of coarse grained models of

liquids and biomolecules. Such models can be used to simulate molecular systems on long time scales. He has also used mode coupling theory to describe and interpret experiments on rotational relaxation in supercooled liquids and nematogens, in collaboration with Professor Michael Fayer of the Stanford Chemistry Department.

## ACADEMIC APPOINTMENTS

- Emeritus Faculty, Acad Council, Chemistry

## ADMINISTRATIVE APPOINTMENTS

- Chair, Stanford University Department of Chemistry, (2002-2005)
- Associate Dean for Natural Sciences, Stanford University School of Humanities and Sciences, (1996-1999)
- David Mulvane Ehrsam and Edward Curtis Franklin Professor in Chemistry, Stanford University, (1994- present)
- Acting Director, Stanford University Center for Materials Research, (1994-1995)
- Deputy Director, Stanford University Center for Materials Research, (1989-1995)
- Co-director, Stanford University Center for Materials Research, (1988-1989)
- Visiting Professor of Chemistry, Columbia University, (1981-1982)
- Professor of Chemistry, Stanford University, (1980- present)
- Associate Professor of Chemistry, Stanford University, (1974-1980)
- Assistant Professor of Chemistry, Stanford University, (1968-1974)
- Junior Fellow, Harvard University Society of Fellows, (1965-1968)

## HONORS AND AWARDS

- Theoretical Chemistry Award, American Chemical Society (2006)
- Dean's Award for Distinguished Teaching, Stanford University (1992)
- Fellow, American Academy of Arts and Sciences (1992)
- Member, National Academy of Sciences (1992)
- Fellow, American Association for the Advancement of Science (1991)
- Joel Henry Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids, American Chemical Society (1988)
- Fellow, American Physical Society (1984)
- John Simon Guggenheim Fellowship, John Simon Guggenheim Foundation (1976-77)
- University Fellow, Stanford University (1975-78)
- Walter J. Gores Award for Excellence in Teaching, Stanford University (1973)
- Sloan Foundation Fellow, Alfred P. Sloan Foundation (1972-74)

## BOARDS, ADVISORY COMMITTEES, PROFESSIONAL ORGANIZATIONS

- Member, Editorial Board, Proceedings of the National Academy of Sciences (2001 - 2005)
- Member, Board on Chemical Sciences and Technology, National Research Council (1995 - 1998)
- Member, Panel on Mathematical Challenges from Computational Chemistry, National Research Council (1994 - 1994)
- Chairman, Gordon Research Conference on the Physics and Chemistry of Liquids (1991 - 1991)
- Vice-chairman, Gordon Research Conference on the Physics and Chemistry of Liquids (1989 - 1989)
- Chairman, Allocation Committee, San Diego Supercomputer Center (1988 - 1989)
- Member, Advisory Board, Journal of Physical Chemistry (1987 - 1992)
- Member, Editorial Board, Chemical Physics (1986 - 1997)
- Member, Allocation Committee, San Diego Supercomputer Center (1986 - 1989)

- Chairman, ACS Physical Chemistry Division (1986 - 1986)
- Chairman Elect and Program Chairman, ACS Physical Chemistry Division (1985 - 1986)
- Member, Editorial Board, Journal of Chemical Physics (1984 - 1986)
- Vice-chair, ACS Physical Chemistry Division (1984 - 1985)
- Member, Editorial Committee, Annual Review of Physical Chemistry (1983 - 1987)

## PROFESSIONAL EDUCATION

- Junior Fellow, Society of Fellows, Harvard University , Statistical mechanics (1968)
- PhD, Massachusetts Institute of Technology , Physical Chemistry (1966)
- BS, Massachusetts Institute of Technology , Chemistry (1962)

## Teaching

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### COURSES

#### 2021-22

- Science in the News: CHEM 25N (Aut)

#### 2020-21

- Science in the News: CHEM 25N (Aut)

## Publications

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### PUBLICATIONS

- **Dynamic force matching: Construction of dynamic coarse-grained models with realistic short time dynamics and accurate long time dynamics** *JOURNAL OF CHEMICAL PHYSICS*  
Davtyan, A., Voth, G. A., Andersen, H. C.  
2016; 145 (22)
- **Critical Slowing of Density Fluctuations Approaching the Isotropic-Nematic Transition in Liquid Crystals: 2D IR Measurements and Mode Coupling Theory.** *journal of physical chemistry. B*  
Sokolowsky, K. P., Bailey, H. E., Hoffman, D. J., Andersen, H. C., Fayer, M. D.  
2016; 120 (28): 7003-7015
- **Dynamic force matching: A method for constructing dynamical coarse-grained models with realistic time dependence** *JOURNAL OF CHEMICAL PHYSICS*  
Davtyan, A., Dama, J. F., Voth, G. A., Andersen, H. C.  
2015; 142 (15)
- **A diagrammatic kinetic theory of density fluctuations in simple liquids in the overdamped limit. I. A long time scale theory for high density** *JOURNAL OF CHEMICAL PHYSICS*  
Pilkiewicz, K. R., Andersen, H. C.  
2014; 140 (15)
- **A diagrammatic kinetic theory of density fluctuations in simple liquids in the overdamped limit. II. The one-loop approximation** *JOURNAL OF CHEMICAL PHYSICS*  
Pilkiewicz, K. R., Andersen, H. C.  
2014; 140 (15)
- **Modified scaling principle for rotational relaxation in a model for suspensions of rigid rods** *JOURNAL OF CHEMICAL PHYSICS*  
Tse, Y. S., Andersen, H. C.  
2013; 139 (4)
- **The multiscale coarse-graining method. IX. A general method for construction of three body coarse-grained force fields** *JOURNAL OF CHEMICAL PHYSICS*  
Das, A., Andersen, H. C.

2012; 136 (19)

- **The multiscale coarse-graining method. X. Improved algorithms for constructing coarse-grained potentials for molecular systems** *JOURNAL OF CHEMICAL PHYSICS*

Das, A., Lu, L., Andersen, H. C., Voth, G. A.

2012; 136 (19)

- **The multiscale coarse-graining method. VIII. Multiresolution hierarchical basis functions and basis function selection in the construction of coarse-grained force fields** *JOURNAL OF CHEMICAL PHYSICS*

Das, A., Andersen, H. C.

2012; 136 (19)

- **A lattice model of the translational dynamics of nonrotating rigid rods** *JOURNAL OF CHEMICAL PHYSICS*

Tse, Y. S., Andersen, H. C.

2012; 136 (2)

- **A Bayesian method for construction of Markov models to describe dynamics on various time-scales** *JOURNAL OF CHEMICAL PHYSICS*

Rains, E. K., Andersen, H. C.

2010; 133 (14)

- **Statistical mechanical basis of coarse graining**

Das, A., Andersen, H. C.

AMER CHEMICAL SOC.2010

- **The multiscale coarse-graining method. V. Isothermal-isobaric ensemble** *JOURNAL OF CHEMICAL PHYSICS*

Das, A., Andersen, H. C.

2010; 132 (16)

- **Efficient, Regularized, and Scalable Algorithms for Multiscale Coarse-Graining** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*

Lu, L., Izvekov, S., Das, A., Andersen, H. C., Voth, G. A.

2010; 6 (3): 954-965

- **Kinetic theories of dynamics and persistent caging in a one-dimensional lattice gas** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*

Abel, S. M., Tse, Y. S., Andersen, H. C.

2009; 106 (36): 15142-15147

- **The multiscale coarse-graining method. III. A test of pairwise additivity of the coarse-grained potential and of new basis functions for the variational calculation** *JOURNAL OF CHEMICAL PHYSICS*

Das, A., Andersen, H. C.

2009; 131 (3)

- **Scaling Analysis of Dynamic Heterogeneity in a Supercooled Lennard-Jones Liquid** *PHYSICAL REVIEW LETTERS*

Stein, R. S., Andersen, H. C.

2008; 101 (26)

- **The multiscale coarse-graining method. II. Numerical implementation for coarse-grained molecular models** *JOURNAL OF CHEMICAL PHYSICS*

Noid, W. G., Liu, P., Wang, Y., Chu, J., Ayton, G. S., Izvekov, S., Andersen, H. C., Voth, G. A.

2008; 128 (24)

- **The multiscale coarse-graining method. I. A rigorous bridge between atomistic and coarse-grained models** *JOURNAL OF CHEMICAL PHYSICS*

Noid, W. G., Chu, J., Ayton, G. S., Krishna, V., Izvekov, S., Voth, G. A., Das, A., Andersen, H. C.

2008; 128 (24)

- **A diagrammatic formulation of the kinetic theory of fluctuations in equilibrium classical fluids. VI. Binary collision approximations for the memory function for self-correlation functions** *JOURNAL OF CHEMICAL PHYSICS*

Noah-Vanhoucke, J. E., Andersen, H. C.

2007; 127 (6)

- **A mode coupling theory description of the short- and long-time dynamics of nematogens in the isotropic phase** *JOURNAL OF CHEMICAL PHYSICS*

Li, J., Cang, H., ANDERSEN, H. C., Fayer, M. D.

2006; 124 (1)

- **Diagrammatic formulation of the kinetic theory of fluctuations in equilibrium classical fluids. V. The short time approximation for the memory function** *JOURNAL OF PHYSICAL CHEMISTRY B*

Ranganathan, M., ANDERSEN, H. C.

2005; 109 (45): 21437-21444

- **Boson peak in supercooled liquids: Time domain observations and mode coupling theory** *JOURNAL OF CHEMICAL PHYSICS*

Cang, H., Li, J., ANDERSEN, H. C., Fayer, M. D.

2005; 123 (6)

- **Molecular dynamics studies of heterogeneous dynamics and dynamic crossover in supercooled atomic liquids** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*

Andersen, H. C.

2005; 102 (19): 6686-6691

- **Tests of an approximate scaling principle for dynamics of classical fluids** *JOURNAL OF PHYSICAL CHEMISTRY B*

Young, T., Andersen, H. C.

2005; 109 (7): 2985-2994

- **A diagrammatic formulation of the kinetic theory of fluctuations in equilibrium classical fluids. IV. The short time behavior of the memory function** *JOURNAL OF CHEMICAL PHYSICS*

Ranganathan, M., Andersen, H. C.

2004; 121 (3): 1243-1257

- **A diagrammatic formulation of the kinetic theory of fluctuations in equilibrium classical fluids. II. Equations of motion of the fluctuation fields and their diagrammatic solution** *JOURNAL OF PHYSICAL CHEMISTRY B*

Andersen, H. C.

2003; 107 (37): 10226-10233

- **Diagrammatic formulation of the kinetic theory of fluctuations in equilibrium classical fluids. III. Cluster analysis of the renormalized interactions and a second diagrammatic representation of the correlation functions** *JOURNAL OF PHYSICAL CHEMISTRY B*

ANDERSEN, H. C.

2003; 107 (37): 10234-10242

- **Dynamical corrections to quantum transition state theory** *JOURNAL OF CHEMICAL PHYSICS*

Cheney, B. G., Andersen, H. C.

2003; 118 (21): 9542-9551

- **A scaling principle for the dynamics of density fluctuations in atomic liquids** *JOURNAL OF CHEMICAL PHYSICS*

Young, T., ANDERSEN, H. C.

2003; 118 (8): 3447-3450

- **A diagrammatic theory of time correlation functions of facilitated kinetic Ising models** *JOURNAL OF CHEMICAL PHYSICS*

Pitts, S. J., ANDERSEN, H. C.

2001; 114 (3): 1101-1114

- **Facilitated spin models, mode coupling theory, and ergodic-nonergodic transitions** *JOURNAL OF CHEMICAL PHYSICS*

Pitts, S. J., Young, T., ANDERSEN, H. C.

2000; 113 (19): 8671-8679

- **The meaning of the irreducible memory function in stochastic theories of dynamics with detailed balance** *JOURNAL OF CHEMICAL PHYSICS*

Pitts, S. J., ANDERSEN, H. C.

2000; 113 (10): 3945-3950

- **Functional and graphical methods for classical statistical dynamics. I. A formulation of the Martin-Siggia-Rose method** *JOURNAL OF MATHEMATICAL PHYSICS*

ANDERSEN, H. C.

2000; 41 (4): 1979-2020

- **Local parabolic reference approximation of thermal Feynman path integrals in quantum Monte Carlo simulations** *JOURNAL OF CHEMICAL PHYSICS*

- Chao, C. E., ANDERSEN, H. C.  
1997; 107 (23): 10121-10130
- **Dynamics of a supercooled Lennard-Jones system: Qualitative and quantitative tests of mode-coupling theory** *PROGRESS OF THEORETICAL PHYSICS SUPPLEMENT*  
Kob, W., Nauroth, M., ANDERSEN, H. C.  
1997: 35-42
  - **Observation of a two-stage melting transition in two dimensions** *PHYSICAL REVIEW E*  
Bagchi, K., ANDERSEN, H. C., Swope, W.  
1996; 53 (4): 3794-3803
  - **Properties of quantum transition state theory and its corrections** *JOURNAL OF PHYSICAL CHEMISTRY*  
Hansen, N. F., ANDERSEN, H. C.  
1996; 100 (4): 1137-1143
  - **Computer simulation study of the melting transition in two dimensions** *PHYSICAL REVIEW LETTERS*  
Bagchi, K., ANDERSEN, H. C., Swope, W.  
1996; 76 (2): 255-258
  - **TESTING MODE-COUPLING THEORY FOR A SUPERCOOLED BINARY LENNARD-JONES MIXTURE .2. INTERMEDIATE SCATTERING FUNCTION AND DYNAMIC SUSCEPTIBILITY** *PHYSICAL REVIEW E*  
Kob, W., ANDERSEN, H. C.  
1995; 52 (4): 4134-4153
  - **TESTING MODE-COUPLING THEORY FOR A SUPERCOOLED BINARY LENNARD-JONES MIXTURE - THE VAN HOVE CORRELATION-FUNCTION** *PHYSICAL REVIEW E*  
Kob, W., ANDERSEN, H. C.  
1995; 51 (5): 4626-4641
  - **A COMPUTER-SIMULATION METHOD FOR THE CALCULATION OF CHEMICAL-POTENTIALS OF LIQUIDS AND SOLIDS USING THE BICANONICAL ENSEMBLE** *JOURNAL OF CHEMICAL PHYSICS*  
Swope, W. C., ANDERSEN, H. C.  
1995; 102 (7): 2851-2863
  - **A NEW FORMULATION OF QUANTUM TRANSITION-STATE THEORY FOR ADIABATIC RATE CONSTANTS** *JOURNAL OF CHEMICAL PHYSICS*  
Hansen, N. F., ANDERSEN, H. C.  
1994; 101 (7): 6032-6037
  - **SCALING BEHAVIOR IN THE BETA-RELAXATION REGIME OF A SUPERCOOLED LENNARD-JONES MIXTURE** *PHYSICAL REVIEW LETTERS*  
Kob, W., ANDERSEN, H. C.  
1994; 73 (10): 1376-1379
  - **SCALING BEHAVIOR IN THE DYNAMICS OF A SUPERCOOLED LENNARD-JONES MIXTURE** *NUOVO CIMENTO DELLA SOCIETÀ ITALIANA DI FISICA D-CONDENSED MATTER ATOMIC MOLECULAR AND CHEMICAL PHYSICS FLUIDS PLASMAS BIOPHYSICS*  
Kob, W., ANDERSEN, H. C.  
1994; 16 (8): 1291-1295
  - **A NEW FORMULATION OF THE HARTREE-FOCK-ROOCHAAN METHOD FOR ELECTRONIC-STRUCTURE CALCULATIONS ON CRYSTALS** *JOURNAL OF CHEMICAL PHYSICS*  
Hammes-Schiffer, S., ANDERSEN, H. C.  
1994; 101 (1): 375-393
  - **KINETIC LATTICE-GAS MODEL OF CAGE EFFECTS IN HIGH-DENSITY LIQUIDS AND A TEST OF MODE-COUPLING THEORY OF THE IDEAL-GLASS TRANSITION** *PHYSICAL REVIEW E*  
Kob, W., ANDERSEN, H. C.  
1993; 48 (6): 4364-4377
  - **THE ADVANTAGES OF THE GENERAL HARTREE-FOCK METHOD FOR FUTURE COMPUTER-SIMULATION OF MATERIALS** *JOURNAL OF CHEMICAL PHYSICS*

- Hammes-Schiffer, S., ANDERSEN, H. C.  
1993; 99 (3): 1901-1913
- **ABINITIO AND SEMIEMPIRICAL METHODS FOR MOLECULAR-DYNAMICS SIMULATIONS BASED ON GENERAL HARTREE-FOCK THEORY JOURNAL OF CHEMICAL PHYSICS**  
Hammes-Schiffer, S., ANDERSEN, H. C.  
1993; 99 (1): 523-532
  - **INTERATOMIC POTENTIALS AND THE PHASE-DIAGRAM OF XE/PT(111) JOURNAL OF CHEMICAL PHYSICS**  
Rejto, P. A., ANDERSEN, H. C.  
1993; 98 (9): 7636-7647
  - **RELAXATION DYNAMICS IN A LATTICE-GAS - A TEST OF THE MODE-COUPLING THEORY OF THE IDEAL GLASS-TRANSITION PHYSICAL REVIEW E**  
Kob, W., ANDERSEN, H. C.  
1993; 47 (5): 3281-3302
  - **THERMODYNAMICS, STATISTICAL THERMODYNAMICS, AND COMPUTER-SIMULATION OF CRYSTALS WITH VACANCIES AND INTERSTITIALS PHYSICAL REVIEW A**  
Swope, W. C., ANDERSEN, H. C.  
1992; 46 (8): 4539-4548
  - **MOLECULAR-DYNAMICS SIMULATION OF SILICA LIQUID AND GLASS JOURNAL OF CHEMICAL PHYSICS**  
DELLAVALLE, R. G., ANDERSEN, H. C.  
1992; 97 (4): 2682-2689
  - **TEST OF A PAIRWISE ADDITIVE IONIC POTENTIAL MODEL FOR SILICA JOURNAL OF CHEMICAL PHYSICS**  
DELLAVALLE, R. G., ANDERSEN, H. C.  
1991; 94 (7): 5056-5060
  - **INTERATOMIC POTENTIAL FOR SILICON CLUSTERS, CRYSTALS, AND SURFACES PHYSICAL REVIEW B**  
BOLDING, B. C., ANDERSEN, H. C.  
1990; 41 (15): 10568-10585
  - **A REACTIVE-FLUX THEORY OF CHEMICAL SURFACE-DIFFUSION JOURNAL OF CHEMICAL PHYSICS**  
Rejto, P. A., ANDERSEN, H. C.  
1990; 92 (10): 6217-6224
  - **10(6)-PARTICLE MOLECULAR-DYNAMICS STUDY OF HOMOGENEOUS NUCLEATION OF CRYSTALS IN A SUPERCOOLED ATOMIC LIQUID PHYSICAL REVIEW B**  
Swope, W. C., ANDERSEN, H. C.  
1990; 41 (10): 7042-7054
  - **LOW-TEMPERATURE APPROXIMATIONS FOR FEYNMAN PATH-INTEGRALS AND THEIR APPLICATIONS IN QUANTUM EQUILIBRIUM AND DYNAMIC PROBLEMS JOURNAL OF CHEMICAL PHYSICS**  
Mak, C. H., ANDERSEN, H. C.  
1990; 92 (5): 2953-2965
  - **ICOSAHEDRAL ORDERING IN THE LENNARD-JONES LIQUID AND GLASS PHYSICAL REVIEW LETTERS**  
Jonsson, H., ANDERSEN, H. C.  
1988; 60 (22): 2295-2298
  - **MONTE-CARLO STUDIES OF DIFFUSION ON INHOMOGENEOUS SURFACES JOURNAL OF CHEMICAL PHYSICS**  
Mak, C. H., ANDERSEN, H. C., George, S. M.  
1988; 88 (6): 4052-4061
  - **MOLECULAR-DYNAMICS STUDY OF MELTING AND FREEZING OF SMALL LENNARD-JONES CLUSTERS JOURNAL OF PHYSICAL CHEMISTRY**  
Honeycutt, J. D., ANDERSEN, H. C.  
1987; 91 (19): 4950-4963

- **MOLECULAR-DYNAMICS COMPUTER-SIMULATION OF AMORPHOUS MOLYBDENUM-GERMANIUM ALLOYS** *PHYSICAL REVIEW B*  
Ding, K., ANDERSEN, H. C.  
1987; 36 (5): 2675-2686
- **THEORETICAL-STUDY OF THE LOCALIZATION-DELOCALIZATION TRANSITION IN AMORPHOUS MOLYBDENUM-GERMANIUM ALLOYS** *PHYSICAL REVIEW B*  
Ding, K., ANDERSEN, H. C.  
1987; 36 (5): 2687-2694
- **MOLECULAR-DYNAMICS SIMULATION OF AMORPHOUS-GERMANIUM** *PHYSICAL REVIEW B*  
Ding, K. J., ANDERSEN, H. C.  
1986; 34 (10): 6987-6991
- **TRUNCATION OF COULOMBIC INTERACTIONS IN COMPUTER-SIMULATIONS OF LIQUIDS** *JOURNAL OF CHEMICAL PHYSICS*  
Linse, P., ANDERSEN, H. C.  
1986; 85 (5): 3027-3041
- **SMALL SYSTEM SIZE ARTIFACTS IN THE MOLECULAR-DYNAMICS SIMULATION OF HOMOGENEOUS CRYSTAL NUCLEATION IN SUPERCOOLED ATOMIC LIQUIDS** *JOURNAL OF PHYSICAL CHEMISTRY*  
Honeycutt, J. D., ANDERSEN, H. C.  
1986; 90 (8): 1585-1589
- **MOLECULAR-DYNAMICS STUDY OF THE HYDROPHOBIC INTERACTION IN AN AQUEOUS-SOLUTION OF KRYPTON** *JOURNAL OF PHYSICAL CHEMISTRY*  
Watanabe, K., ANDERSEN, H. C.  
1986; 90 (5): 795-802
- **FACILITATED KINETIC ISING-MODELS AND THE GLASS-TRANSITION** *JOURNAL OF CHEMICAL PHYSICS*  
FREDRICKSSON, G. H., ANDERSEN, H. C.  
1985; 83 (11): 5822-5831
- **MACROMOLECULAR PAIR CORRELATION-FUNCTIONS FROM FLUORESCENCE DEPOLARIZATION EXPERIMENTS** *JOURNAL OF POLYMER SCIENCE PART B-POLYMER PHYSICS*  
FREDRICKSSON, G. H., ANDERSEN, H. C., Frank, C. W.  
1985; 23 (3): 591-599
- **A COMPARISON OF THE MOLECULAR-DYNAMICS METHOD AND ENERGY MINIMIZATION METHODS FOR MODELING THE STRUCTURE OF AMORPHOUS METALS** *JOURNAL OF NON-CRYSTALLINE SOLIDS*  
GRABOW, M. H., ANDERSEN, H. C.  
1985; 75 (1-3): 225-236
- **EFFECTS OF 3-BODY INTERACTIONS ON THE STRUCTURE OF CLUSTERS** *SURFACE SCIENCE*  
BLAISTENBAROJAS, E., ANDERSEN, H. C.  
1985; 156 (JUN): 548-555
- **HOPPING TRANSPORT ON A RANDOMLY SUBSTITUTED LATTICE FOR LONG-RANGE AND NEAREST NEIGHBOR INTERACTIONS** *JOURNAL OF CHEMICAL PHYSICS*  
Loring, R. F., ANDERSEN, H. C., Fayer, M. D.  
1984; 80 (11): 5731-5744
- **HOPPING TRANSPORT ON A RANDOMLY SUBSTITUTED LATTICE IN THE PRESENCE OF DILUTE DEEP TRAPS** *CHEMICAL PHYSICS*  
Loring, R. F., ANDERSEN, H. C., Fayer, M. D.  
1984; 85 (1): 149-164
- **MOLECULAR-DYNAMICS SIMULATIONS OF A SUPERCOOLED MONATOMIC LIQUID AND GLASS** *JOURNAL OF PHYSICAL CHEMISTRY*  
Fox, J. R., ANDERSEN, H. C.  
1984; 88 (18): 4019-4027
- **KINETIC ISING-MODEL OF THE GLASS-TRANSITION** *PHYSICAL REVIEW LETTERS*  
FREDRICKSON, G. H., ANDERSEN, H. C.

1984; 53 (13): 1244-1247

• **THE EFFECT OF PERIODIC BOUNDARY-CONDITIONS ON HOMOGENEOUS NUCLEATION OBSERVED IN COMPUTER-SIMULATIONS** *CHEMICAL PHYSICS LETTERS*

Honeycutt, J. D., ANDERSEN, H. C.

1984; 108 (6): 535-538

• **A MOLECULAR-DYNAMICS METHOD FOR CALCULATING THE SOLUBILITY OF GASES IN LIQUIDS AND THE HYDROPHOBIC HYDRATION OF INERT-GAS ATOMS IN AQUEOUS-SOLUTION** *JOURNAL OF PHYSICAL CHEMISTRY*

Swope, W. C., ANDERSEN, H. C.

1984; 88 (26): 6548-6556

• **ELECTRONIC EXCITED-STATE TRANSPORT AND TRAPPING ON POLYMER-CHAINS** *MACROMOLECULES*

FREDRICKSON, G. H., ANDERSEN, H. C., Frank, C. W.

1984; 17 (1): 54-59

• **ELECTRONIC EXCITATION TRANSPORT AS A PROBE OF CHAIN FLEXIBILITY** *MACROMOLECULES*

FREDRICKSON, G. H., ANDERSEN, H. C., Frank, C. W.

1984; 17 (8): 1496-1499

• **THE ROLE OF LONG RANGED FORCES IN DETERMINING THE STRUCTURE AND PROPERTIES OF LIQUID WATER** *JOURNAL OF CHEMICAL PHYSICS*

ANDREA, T. A., Swope, W. C., ANDERSEN, H. C.

1983; 79 (9): 4576-4584

• **VANDERWAALS PICTURE OF LIQUIDS, SOLIDS, AND PHASE-TRANSFORMATIONS** *SCIENCE*

CHANDLER, D., WEEKS, J. D., ANDERSEN, H. C.

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• **CLUSTER EXPANSIONS FOR HYDROGEN-BONDED FLUIDS .3. WATER** *JOURNAL OF CHEMICAL PHYSICS*

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1983; 78 (4): 1962-1979

• **A THEORY OF THE ANOMALOUS THERMODYNAMIC PROPERTIES OF LIQUID WATER** *JOURNAL OF CHEMICAL PHYSICS*

DAHL, L. W., ANDERSEN, H. C.

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• **ELECTRONIC EXCITED-STATE TRANSPORT ON ISOLATED POLYMER-CHAINS** *MACROMOLECULES*

FREDRICKSON, G. H., ANDERSEN, H. C., Frank, C. W.

1983; 16 (9): 1456-1464

• **EXCITATION TRANSPORT ON SUBSTITUTIONALLY DISORDERED LATTICES**

Loring, R. F., ANDERSEN, H. C., Fayer, M. D.

AMER INST PHYSICS.1983: 1389-89

• **ELECTRONIC EXCITED-STATE TRANSPORT AND TRAPPING AS A PROBE OF INTRAMOLECULAR POLYMER STRUCTURE** *JOURNAL OF CHEMICAL PHYSICS*

FREDRICKSON, G. H., ANDERSEN, H. C., Frank, C. W.

1983; 79 (7): 3572-3580

• **EXCITATION TRANSPORT ON SUBSTITUTIONALLY DISORDERED LATTICES** *PHYSICAL REVIEW LETTERS*

Loring, R. F., ANDERSEN, H. C., Fayer, M. D.

1983; 50 (17): 1324-1327

• **RATTLE - A VELOCITY VERSION OF THE SHAKE ALGORITHM FOR MOLECULAR-DYNAMICS CALCULATIONS** *JOURNAL OF COMPUTATIONAL PHYSICS*

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