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- Dezember 1992 des Landes Rheinland-Pfalz
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- Mai 1986 - Vorsitzender des Koordinationsausschusses des Material-
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- seit Februar 1987 „Adjunct Professor“ am Center for Simulational Physics,
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1. Juli 1987 - Sprecher des Sonderforschungsbereichs 262 der
31. Dezember 2001 Deutschen Forschungsgemeinschaft („Glaszustand und
Glasübergang nichtmetallischer amorpher Materialien“)
- Juli 1987 - Mitglied des „Wissenschaftlichen Rats“
Juli 1995 des HLRZ (Höchstleistungsrechenzentrum) in Jülich
- 1988 – 1990 und Mitglied der IUPAP Commission C3
1996 – 1999 „Thermodynamics and Statistical Physics“ und des
DNK (Deutsches Nationales Komitee für IUPAP)
29. November 1988 Erhalt eines Rufes zum Direktor an das
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20. Juni 1989 Ernennung zum Auswärtigen Mitglied
der Max Planck Gesellschaft
12. Mai 1992 Ernennung zum Korrespondierenden Mitglied der
Österreichischen Akademie der Wissenschaften, Wien
24. März 1993 Max-Planck-Medaille 1993 erhalten von der
Deutschen Physikalischen Gesellschaft (DPG)
- 1999 – 2002 Vorsitzender der IUPAP-Kommission C3 „Thermodynamics
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Council“ der IUPAP

2001	Auszeichnung als „Highly Cited Researcher“ durch das Institute for Scientific Information (ISI), Philadelphia, USA (“Top-100” List in Science Citation Index of Physics, 1981-1999)
6. September 2001	Berni J. Alder CECAM Prize (auf dem Gebiet der Computerorientierten Physik) der EPS
21. Februar 2003	Ernennung zum Mitglied der Akademie der Wissenschaften und der Literatur, Mainz
15. Januar 2003 - 30. April 2005	Dekan des Fachbereichs Physik der Johannes-Gutenberg Universität Mainz
24. Januar 2003	Staudinger-Durrer-Preis der ETH Zürich
2. November 2005	Ernennung zum Auswärtigen Mitglied der Bulgarischen Akademie der Wissenschaften, Sofia, Bulgarien
1. Oktober 2003 – 30. September 2006	Mitglied des Universitätsrats der Universität Stuttgart
seit 2006	Mitglied „ehrenhalber“ des britischen Instituts of Physics (IOP)
24. Januar 2007	Verleihung des Dr. h.c. in Chemie der Maria-Curie-Sklodowska Universität Lublin, Polen
11. Juli 2007	Verleihung der Boltzmann-Medaille der IUPAP
23. Oktober 2007	Verleihung des Gutenberg Fellowships der Universität Mainz
2008 - 2013	Mitglied im wissenschaftlichen Beratungsgremium des Max Planck Institutes für „Kolloid und Grenzflächen-Forschung“
seit 2009	Mitglied im „Rat für Technologie, Rheinland-Pfalz“
23. September 2009	Verleihung des „Lennard Jones Lecture Awards“ durch die Royal Society of Chemistry, London
seit 2010 - 2012	Mitglied des “Scientific Steering Committee of the Partnership for Advanced Computing in Europe (PRACE)”
2011	Stellvertretender Vorsitzender des wissenschaftlichen Rates des John von Neumann Institutes für Computing (NIC), Jülich
April 2011	Mitglied der Nationalen Akademie der Wissenschaften, Leopoldina, Halle
2012 - 2017	Vorsitzender des wissenschaftlicher Rates des John von Neumann Insitutes für Computing (NIC) Jülich
2012 – 2017	Vize-Präsident des „Steering Committee’s“ des Gauss Centers für Computing
seit 1. April 2012	Professor „emeritus“

- | | |
|--------------------|--|
| 19. September 2012 | Ehrenmedaille „Marin Drinov“ der bulgarischen Akademie der Wissenschaften |
| 30. Januar 2013 | Ehrendoktorwürde der Mathematisch-Naturwissenschaftlichen Fakultät der Heinrich-Heine-Universität Düsseldorf für bedeutende Beiträge zum Sonderforschungsbereich TR6 „Physik kolloidaler Dispersionen in äußeren Feldern |
| seit 1. Jan 2018 | Stellvertretender Vorsitzender des John von Neumanns Institute für Computer (NIC) Jülich |

Supervision of Ph.D. theses/Betreuung von Doktorarbeiten

Prior to the “Habilitation” (1973), only an “inofficial” Ph.D. advisor status was possible for the following two cases:

- (i) Volker Wildpaner “Berechnung der Magnetisierung um Gitterfehler in einem Heisenberg Ferromagneten” Technische Hochschule Wien, 1972
- (ii) Heiner-Müller-Krumbhaar “Bestimmung kritischer Exponenten am Heisenberg-Ferromagneten mit einem selbstkonsistenten Monte-Carlo Verfahren” Physik-Department, Technische Hochschule München, 1972

A) Universität des Saarlandes, Saarbrücken

1. Artur Baumgärtner “Die verallgemeinerte kinetische Ising-Kette: Ein Modell für die Dynamik von Biopolymeren” 1977
2. Claudia Billotet “Nichtlineare Relaxation bei Phasenübergängen: Eine Ginzburg-Landau Theorie mit Fluktuationen” 1979
3. Rüdiger Kretschmer “Kritisches Verhalten und Oberflächeneffekte von Systemen mit lang- und kurzreichweitigen Wechselwirkungen: Phänomenologische Theorie und Monte Carlo Simulation” 1979
4. Ingo Morgenstern “Ising Systeme mit eingefrorener Unordnung in zwei Dimensionen” 1980

B) Universität zu Köln

5. Kurt Kremer “Untersuchungen zur statistischen Mechanik von linearen Polymeren unter verschiedenen Bedingungen” 1983
6. Jozsef Reger “Untersuchungen zur statistischen Mechanik von Spingläsern” 1985

C) Johannes Gutenberg Universität

7. Ingeborg Schmidt “Oberflächenanreicherung und Wettingphasenübergänge in Polymermischungen” 1986
8. Jannis Batoulis “Monte Carlo Simulation von Sternpolymeren” 1987

9. Hans-Otto Carmesin "Modellierung von Orientierungsgläsern" 1988
10. Wolfgang Paul "Theoretische Untersuchungen zur Kinetik von Phasenübergängen erster Ordnung"
11. Manfred Scheucher "Phasenverhalten und Grundzustandseigenschaften kurzreichweitiger Pottsgläser" 1990
12. Hans-Peter Wittmann "Monte Carlo Simulationen des Glasübergangs von Polymerschmelzen im Rahmen des Bondfluktuationsalgorithmus" 1991
13. Burkhard Dünweg "Molekular-dynamik-Untersuchungen zur Dynamik von Polymerketten in verdünnter Lösung" 1991
14. Friederike Schmid "Volumen-Grenzflächeneigenschaften von Modellen kubisch-raumzentrierter binärer Legierungen: Untersuchung mittels Monte Carlo Simulation" 1991
15. Hans-Peter Deutsch "Computer-Simulation von Polymer-Mischungen" 1991
16. Werner Helbing "Quanten Monte Carlo Simulation eines Rotatormoleküls" 1992
17. Dominik Marx "Entwicklung von Pfadintegral Monte Carlo Methoden für adsorbierte Moleküle mit inneren Quantenfreiheitsgraden" 1992
18. Gernot Schreider "Hochtemperaturreihenentwicklungen zum geordneten und ungeordneten Potts-Modell" 1993
19. Jörg Baschnagel "Monte Carlo Simulationen des Glasübergangs und Glaszustandes von dichten dreidimensionalen Polymerschmelzen" 1993
20. Marco d'Onorio de Meo "Monte Carlo Methoden zur Untersuchung reiner und verdünnter Ferromagnete mit kontinuierlichen Spins" 1993
21. Marcus Müller "Monte Carlo Simulation zur Thermodynamik und Struktur von Polymer-Mischungen" 1994
22. Klaus Eichhorn "Pottsmodelle zu Zufallfeldern" 1995
23. Frank M. Haas "Monolagen steifer Kettenmoleküle auf Oberflächen. Eine Monte Carlo Simulationsuntersuchung" 1995
24. Matthias Wolfigardt "Monte Carlo Simulation zur Zustandsgleichung glasartiger Polymerschmelzen" 1995
25. Martin H. Müser "Klassische und quantenmechanische Computer Simulationen zur Orientierungsgläsern und Kristallen" 1995
26. Stefan Kappler "Oberflächenspannung und Korrelationslängen im Pottsmodell" 1995
27. Felix S. Schneider "Quanten-Monte-Carlo-Computersimulationsstudie der Dynamik des inneren, quantenmechanischen Freiheitsgrades eines Modell-Fluids in reeller Zeit" 1995
28. Katharina Vollmayr "Abkühlungsabhängigkeiten von strukturellen Gläsern: Eine Computersimulation" 1995

29. Volker Tries "Monte Carlo Simulationen realistischer Polymerschmelzen mit einem vergrößerten Modell" 1996
30. Martina Kreer "Quantenmechanische Anomalien bei Phasenübergängen in 2D: Eine Pfadintegral-Monte-Carlo Studie zu H₂ und O₂ physisorbiert auf Graphit" 1996
31. Bernhard Lobe "Stargraph-Entwicklungen zum geordneten und ungeordneten Potts-Modell und deren Analysen" 1997
32. Stefan Kämmerer "Orientierungsdynamik in einer unterkühlten Flüssigkeit: eine MD-Simulation" 1997
33. Henning Weber "Monte Carlo-Simulationen der Gasdiffusion in Polymermatrizen" 1997
34. Rüdiger Sprengard "Raman-Spektroskopie in Li₂O · Al₂O₃ · SiO₃- Glaskeramiken: Simulation und Kristallspektren und experimentelle Untersuchungen zum Keramisierungsprozeß" 1998
35. Frank F. Haas "Oberflächeninduzierte Unordnung in binären bcc Legierungen" 1998
36. Jürgen Horbach "Molekulardynamiksimulationen zum Glasübergang von Silikatschmelzen" 1998
37. Matthias Presber "Pfadintegral-Monte Carlo Untersuchungen zu Phasenübergängen in molekularen Festkörpern" 1998
38. Christoph Stadler "Monte Carlo Simulation in Langmuir Monolagen" 1998
39. Andres Werner "Untersuchung von Polymer-Grenzflächen mittels Monte Carlo Simulationen" 1998
40. Christoph Bennemann "Untersuchung des thermischen Glasübergangs von Polymerschmelzen mittels Molekular-Dynamik Simulationen" 1999
41. Tobias Gleim "Relaxation einer unterkühlten Lennard-Jones Flüssigkeit" 1999
42. Fathollah Varnik "Molekulardynamik-Simulationen zum Glasübergang in Makromolekularen Filmen" 2000
43. Dirk Olaf Löding "Quantensimulationen physisorbierter Molekülschichten auf Graphit: Phasenübergänge, Quanteneffekte, und Glaseigenschaften" 2000
44. Alexandra Roder "Molekulardynamik-Simulationen zu Oberflächeneigenschaften von Siliziumdioxidschmelzen" 2000
45. Oliver Dillmann "Monte Carlo Simulationen des kritischen Verhaltens von dünnen" Ising Filmen" 2000
46. Harald Lange "Oberflächengebundene flüssigkristalline Polymere in nematischer Lösung: eine Monte Carlo Untersuchung" 2001
47. Peter Scheidler "Dynamik unterkühlter Flüssigkeiten in Filmen und Röhren" 2001
48. Claudio Brangian "Monte Carlo Simulation of Potts-Glasses" 2002
49. Torsten Kreer "Molekulardynamik-Simulation zur Reibung zwischen polymerbeschichteten Oberflächen" 2002

50. Stefan Krushev "Computersimulationen zur Dynamik und Statistik von Polybutatien-schmelzen" 2002
51. Susanne Metzger "Monte Carlo Simulationen zum Adsorptionsverhalten von Homo-Copolymeren" 2002
52. Claus Mischler "Molekulardynamik-Simulation zur Struktur von SiO₂-Oberflächen mit adsorbiertem Wasser" 2002
53. Ellen Reister "Zusammenhang zwischen der Einzelkettendynamik und der Dynamik von Konzentrationsfluktuationen in mehrkomponentigen Polymersystemen: dynamische Mean-Field Theorie und Computersimulation" 2002
54. Anke Winkler "Molekulardynamik-Untersuchungen zur atomistischen Struktur und Dynamik von binären Mischgläsern Na₂O₂ und (Al₂O₃) (2SiO₂)" 2002
55. Martin Aichele "Simulation Studies of Correlation Functions and Relaxation in Polymeric Systems" 2003
56. Peter M. Virnau "Monte Carlo Simulationen zum Phasen- und Keimbildungsverhalten von Polymerlösungen" 2003
57. Daniel Herzbach "Comparison of Model Potentials for Molecular Dynamics Simulation of Crystalline Silica" 2004
58. Hans R. Knoth "Molekular-Dynamik-Simulation zur Untersuchung des Mischalkali-Effekts in silikatischen Gläsern" 2004
59. Florian Krajewski "New path integral simulation algorithms and their application to creep in the quantum sine-Gordon chain" 2004
60. Ben Jesko Schulz "Monte Carlo Simulation of Interface Transitions in Thin Film with Competing Walls" 2004
61. Torsten Stühn "Molekular-Dynamik Computersimulation einer amorph-kristallinen SiO₂ Grenzschicht" 2004
62. Ludger Wenning "Computersimulation zum Phasenverhalten binärer Polymerbürsten" 2004
63. Juan Guillermo Diaz Ochoa "Theoretical investigation of the interaction of a polymer film with a nanoparticle" 2005
64. Federica Rampf "Computer Simulationen zur Strukturbildung von einzelnen Polymerketten" 2005
65. Michael Hawlitzky "Klassische und ab initio Molekulardynamik-Untersuchungen zu Germaniumdioxidschmelzen" 2006
66. Andrea Ricci "Computer Simulations of two-dimensional colloidal crystals in confinement" 2006
67. Antoine Carré "Development of empirical potentials for liquid silica" 2007
68. Svetlana Jungblut "Mixtures of colloidal rods and spheres in bulk and in confinement" 2008

69. Yulia Trukhina “Monte Carlo Simulation of Hard Spherocylinders under confinement”
2009
70. Leonid Spirin “Molecular Dynamics Simulations of sheared brush-like systems”
2010
71. Daniel Reith “Computersimulationen zum Einfluß topologischer Beschränkungen auf
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72. Alexander Winkler “Computer simulations of colloidal fluids in confinement”
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73. David Winter “Computer simulations of slowly relaxing systems in external fields”
2012
74. Dorothea Wilms “Computer simulations of two-dimensional colloidal crystals under
confinement and shear” 2013
75. Benjamin Block “Nucleation Studies on Graphics Processing Units” 2014
76. Fabian Schmitz “Computer Simulations Methods to study Interfacial Tensions: From the
Ising Model to Colloidal Crystals” 2014
77. Antonia Statt “Monte Carlo Simulations of Nucleation of Colloidal Crystals” 2015
78. Peter Koss “Computer Simulations on Homogeneous Nucleation in Crystalline Systems”
2018

Main Research Interests

1. Monte Carlo simulation as a tool of computational statistical mechanics to study phase transitions

A main research goal has been to develop Monte Carlo techniques for the numerical study of classical interacting many body systems, with an emphasis on phase transitions in condensed matter [33,41,76,153,189,205,244,321,491,551,630,970,1132, number refer to the list of publications, see:[publication list Binder](#).] A central obstacle to overcome are finite size effects: Ising and classical Heisenberg ferromagnets [5] exhibit the “finite size tail” in the root mean square magnetization, which is strongly enhanced near the critical point (due to the divergence of correlation length and susceptibility in the thermodynamic limit), leading to finite size rounding and shifting of the transition [16,29]. Combining this starting point with the finite size scaling theory developed by M.E. Fisher at about the same time, numerous promising first studies of phase transitions were given [33,41,75,76,92,103] but the main breakthrough came from a study of the order parameter probability distribution and its fourth order cumulant [135]. For different system sizes the cumulants (studied as function of the proper control parameter, e.g. temperature) intersect at criticality at an (almost) universal value, and this allows an easy and unbiased estimation of the critical point location. This method has helped to study phase transitions and phase diagrams of many model systems and now is widely used by many research groups. A recent extension of this finite-size scaling analysis of phase transitions [1179] has considered the case of first order transitions. While for the case of the order-disorder transition of the q-state Potts model the q-fold degeneracy of the ordered phase leads to a finite-size shift of the transition temperature, proportional to $\ln(q)$, it had been unclear what the analogy of the degeneracy number q is when a continuous symmetry is broken. In [1179] it is argued that $q=\pi$, in the case where a XY-like order parameter occurs. It was also shown that the first and second moments of the order parameter distribution also exhibit unique (universal) intersection points, in addition to the cumulant intersection. Thus, 50 years after the first formulation of finite-size scaling

concepts still gaps in the description needed to be filled. Lattice models for adsorbed monolayers at crystal surfaces have been studied to clarify corresponding experiments (e.g. H on Pd (100) [127], H on Fe (100) [145,154] or CO and N₂ on graphite [398,411]). Lattice models for solid alloys have been used to understand the ordering in Cu-Au alloys [16,124,210,215], of Fe-Al alloys [355,380], and of magnetic ordering of EuS diluted with SrS [86,103,105]. Later finite size scaling methods have also been used to study off-lattice models for the $\alpha - \beta$ phase transition in SiO₂ [676] and the vapor-liquid phase transitions of CO₂ [916] and various liquid mixtures [943] and good agreement with experiment was found. The technique could also be extended to very asymmetric systems, such as the Asakura-Oosawa model for colloid-polymer mixtures [823] and rod-sphere mixtures [910].

Since finite size scaling in its standard formulation needs “hyperscaling” relations between critical exponents to hold (see e.g. [135]), nontrivial generalizations needed to be developed for cases where hyperscaling does not hold, such as model systems in more than 4 space dimensions [184,195,596] and Ising-type systems with quenched random fields (such as colloid-polymer mixtures inside a randomly-branched gel) [883,939,1016]. Other generalizations concern anisotropic critical phenomena [261], e.g. critical wetting transitions [1061,1068,1095], and crossover from one universality class to another [369,524,593], e.g. when the effective interaction range increases the system criticality changes to become mean-field like (an application being binary polymer blends when the chain length of the macromolecules increases [414]). An important task in the study of phase transitions by simulations is the distinction of second order phase transitions from first-order ones, a problem studied in collaboration with David Landau since also the latter are rounded (and possibly shifted) by finite size (e.g. [182,212,262,375,1066]). Some of the “recipes” developed to study phase transitions by simulations using Monte Carlo methods are reviewed in [201,375,656,912]; we also note that finite size scaling concepts are also useful for Molecular Dynamics methods, and then allow also the study of dynamic critical behavior of fluids [801,868,873].

2. Monte Carlo simulation as a tool to study dynamical behavior in condensed matter systems

One can give the Monte Carlo sampling process a dynamic interpretation in terms of a Markovian master equation [24]; on the one hand, one can thus give statistical errors an appropriate interpretation in terms of dynamic correlation functions of the appropriate stochastic model, and understand what the slowest relaxing variables are: e.g., for a fluid these are long wavelength Fourier components of the density, when the fluid is simulated in the canonical ensemble. This “hydrodynamic slowing down” [33,76] was not recognized in the early literature on Monte Carlo simulations of fluids, where the relaxation of the internal energy was advocated to judge the approach to equilibrium. In this way, it also becomes possible to understand that the so-called “statistical inefficiency” of the Monte Carlo algorithm near second-order phase transitions simply reflects critical slowing down, and it is possible to study the latter systematically by Monte Carlo e.g. for finite kinetic Ising models [26,1132], although even with the computer power available in the 21st century this is a demanding task, and thus the early work [26] could not reach a meaningful accuracy. A subtle aspect (that still does not seem to be widely recognized) is the fact that critical slowing down leads to a systematic bias (due to finite time averaging) in the sampling of susceptibilities using fluctuation relations [298]. One also needs to be aware that the latter suffer from a lack of self-averaging [214]. At first-order transitions, rather than critical slowing down one may encounter metastability and hysteresis [33,76], but on the other hand, the decay of metastable states (via nucleation and growth) is an interesting problem, both from the point of view of analytical theory [25], phenomenological theories based on the dynamical evolution of the “droplet” size distribution [53] and via attempts to directly study nucleation kinetic by simulation [27,30]. However, these early studies of nucleation phenomena in kinetic Ising models encountered two basic difficulties: (i) due to by far insufficient computer resources, only nucleation barriers of a few times the thermal energy were accessible. (ii) ambiguities in the definition of “clusters” [51]. Both difficulties could only recently be overcome [1090], showing that only the use of the Swendsen-Wang definition of “physical clusters” allows a consistent description of nucleation phenomena in the Ising model, and then the classical theory of nucleation is compatible with the observations of the kinetics [1153].

The dynamic interpretation of Monte Carlo sampling is the basis for a broad range of kinetic Monte Carlo studies of stochastic processes, such as diffusion in concentrated (and possibly interacting) lattice

gases [126,146,163], surface diffusion [161] and kinetics of domain growth [168,179], and last but not least interdiffusion in alloys [263] and spinodal decomposition of alloys using the vacancy mechanism [297,301,319]. Other groups have taken the subject of kinetic Monte Carlo and developed it to become a powerful tool of computational materials science.

3. Spinodal decomposition and the non-existence of spinodal curves

While generalized nonlinear Cahn-Hilliard type equations for phase separation kinetics could be derived from kinetic Ising models [37], it was emphasized that the critical singularities that result from the linearization of the Cahn-Hilliard equation are a mean-field artefact, and rather one has a gradual and smooth transition between nonlinear spinodal decomposition and nucleation [52,53,68,80,87]. To show this, a phenomenological description of spinodal decomposition in terms of the dynamics of many growing clusters was developed [68,70,80], which also allowed to understand the diffusive growth law for spinodal decomposition in liquid binary mixtures [43], and provided a dynamic scaling concept for the structure factor of phase separating systems [61,68,80]. It was numerically demonstrated by Monte Carlo estimations of small subsystem free energies that the spinodal has a well defined meaning for subsystems with a linear dimension L that is small in comparison with the correlation length [162,181], since the order parameter in such small subsystems always is essentially homogeneous. For large L the distance of the “spinodal” from the coexistence curve decays with the minus 4th power of L (in $d=3$ dimensions). Later this observation was explained via the phenomenological theory for the “droplet evaporation/condensation transition” [750]. The latter has been studied via simulations [966].

It needs to be emphasized that the above results apply for systems with short-range interactions. When the interaction range R diverges, nucleation gets more and more suppressed (since the interfacial free energy is proportional to R), and metastable states still have a large life time rather close to the mean field spinodal [169,219,221]. Similarly, for large R the linearized Cahn theory of spinodal decomposition is predicted to hold in the initial stages, and this has been verified for phase separation of symmetrical polymer mixtures, as reviewed in [288,702]. These Ginzburg criteria [169,219,221] explain why the spinodal is useful for mean field systems but not beyond [1074].

4. Surface critical phenomena, interfaces, and wetting

At the critical point of a ferro- or antiferromagnet critical correlations at a free surface show an anisotropic power law decay, and the critical exponents describing this decay differ from the bulk [19,31,42,48,151,270]. A phenomenological scaling theory for surface critical phenomena could be derived [19,31] in collaboration with Pierre Hohenberg, including scaling laws relating the new critical exponents to each other and to bulk ones, and numerical evidence from both systematic high temperature expansions and simulations was obtained to support this theoretical description. The Monte Carlo simulation method uses periodic boundary conditions throughout to describe bulk systems, but free boundary conditions in one direction (and periodic in the other) are used to study thin magnetic films [29]. Also small (super paramagnetic) particles can be studied [8], where a combination of surface and size effects matters (see also [1082]). In ferroelectrics and dipolar magnets even on the mean field level the description gets more complicated [91,137], due to the fact that depolarizing fields cannot be neglected. For short-range systems, on the other hand, estimations of the critical exponents associated with the “surface-bulk multicritical point” have remained a longstanding challenge [178,276,283,294]. An interesting extension also is needed for surface criticality if the bulk system exhibits a Lifshitz point [590,637], since then the system exhibits anisotropic critical behavior in the bulk. This problem was treated by deriving an appropriate Landau theory from the lattice mean field theory of a semi-infinite ANNNI model. A similar concept was used to describe the dynamics of surface enrichment, deriving the proper boundary conditions at a surface for a Cahn-Hilliard type description from a lattice formulation [325], which also is the starting point to study surface-directed spinodal decomposition [333,348,427,495,559,565,605,668,748,963]. Finally, critical surface induced ordering or disordering at bulk first-order transitions was studied [302,500,618]. Qualitatively, such transitions are understood in terms of the gradual unbinding of an interface between the ordered and disordered phase of the system from a surface, reminiscent of wetting phenomena.

In fact, the understanding of interfaces between coexisting phases has been one of the longstanding research interests as well. It was already realized soon [140] that sampling the size-dependence of the minimum of the distribution of the order parameter that describes the two coexisting phases yields information on the “surface tension” (i.e., the interfacial excess free energy). Originally developed for the Ising model [140] and then for lattice models of polymer mixtures [472], this method has become one of the widely used standard methods to estimate surface tensions at gas-liquid transitions (e.g. [823,916,943], but only recently could the subtle finite size corrections to this method be clarified [1119,1127]).

An interesting property of interfaces is the order parameter profile across the interface [391,392]. In $d=3$ dimensions lattice models can show a roughening transition [260,391], where in the thermodynamic limit the interfacial width diverges. The interfacial width then scales logarithmically with the interfacial area [392,611,669,673,833,968,999], and the mean field (van der Waals, Cahn-Hilliard, etc) concept of an “intrinsic interfacial profile” becomes doubtful. While this logarithmic broadening of the interfacial profile could also be established for solid-fluid interfaces [968,999], in solid-solid interfaces elastic interactions may suppress this broadening [819], yielding a well-defined intrinsic profile again. Particularly interesting are interfaces confined between walls in thin film geometry [555,587,588]; the resulting anomalous dependence of the interfacial width on the film thickness could also be proven to occur in thin films of unmixed polymer blends through appropriate experiments [513,578].

Interfaces confined between parallel walls can also undergo an interface location/delocalization transition [272,442,468,503,571,638,653,659,681,820]. This transition is the analog of the interface unbinding from a surface of a semi-infinite system, i.e. wetting transition, which is a difficult critical phenomenon in the case of short-range forces [206,222,233,277,295,313,353,572,1024,1061,1092]. Interesting interface unbinding transitions were also found in wedges [764,767] and bi-pyramide confinement [815,835], giving rise to unconventional new types of critical phenomena. Also interesting first-order transitions such a capillary condensation [344,356,677] can be studied for systems confined in strips, cylindrical or slit-like pores [275,834,874,1006,1008]. Then also phenomena such as heterogeneous nucleation at walls [967,974,1062] come into play; however, this problem is difficult since it requires consideration of both curvature effects on the interfacial free energy [966,1011,1045,1047,1051] and possible effects due to the line tension [1021,1131,1173]. First steps of a methodology to deal with all these problems via simulations were developed [966,968,1011,1021,1029,1045,1047,1051,1057,1062,1131]. Particularly challenging is the treatment of crystal nucleation from fluid phases, since in general the interface free energy depends on the interface orientation relative to the lattice axes [1135,1137,1138,1166]. A methodology to circumvent this problem was invented [1133,1135], analyzing the equilibrium between a crystal nucleus and surrounding fluid in a finite simulation box, using a new method to sample the fluid chemical potential.

5. Spin glasses and glass-forming fluids

The “standard model” for spin glasses is the Edwards-Anderson model, i.e. an Ising Hamiltonian where the exchange coupling is a random quenched variable, either drawn from a Gaussian distribution or chosen as $\pm J$. First Monte Carlo simulations of this model in $d=2$ dimensions [60,66] showed a cusp-like susceptibility peak similar to experiment; however, now it is known that this peak simply is an effect of the finite (short) observation time, and spin glass-like freezing in $d=2$ occurs at zero temperature only [104,106]. Recursive transfer matrix calculations [104,106] showed that at $T=0$ spin-glass-type correlations exhibit a power law decay with distance in the $\pm J$ model. The spin-glass correlation length and associated susceptibility diverge with power laws of $1/T$ as the temperature T tends to zero [106]. Also a more realistic site disorder model for the insulating spin glasses EuS diluted with SrS was developed, and good agreement with experiment was found [86,105], and critical magnetic fields in spin glasses were discussed [164,171]. Also some aspects of random field Ising models [159,174,421] and random field Potts models [479,521] were considered. Together with Peter Young a comprehensive review on spin glasses was written, encompassing experiments, theory, and simulation; this highly cited paper still is the standard review of the field.

Considering Edwards-Anderson models where spins are replaced by quadrupole moments one obtains models for “quadrupolar glasses” [234,238,250,268,291,306,474,515,567,583,679,691,694,730,766], which can be realized experimentally by diluting molecular crystals with atoms which have no quadrupole moment (e.g. N₂ diluted with Ar, or K(CN) diluted with K Cl [387]). An atomistic model for such a system was simulated in [540], and a detailed review is found in [387].

Also various contributions were made attempting to elucidate the “grand challenge problem” how a supercooled fluid freezes into a glass. First studies were devoted to develop a lattice model for the glass transition of polymers, introducing “frustration” in the bond fluctuation model via energetic preference for long bonds, which “waste” lattice sites for further occupation by monomers [334,374,388,400,405,417,423,433,435,476,493,496,506,528,549,696]. It was shown that much of the experimental phenomenology could be reproduced (stretched relaxation, time-temperature superposition principle, Vogel-Fulcher relation describing the increase of the structural relaxation time, and evidence in favor of the mode coupling theory as a description of the initial stages of slowing down). Many of these features could also be demonstrated by molecular dynamics simulations of a more realistic off-lattice bead spring model of macromolecules [577,598,600,617,628,708,709], including an analysis of the surface effects on the glass transition in thin polymer films [708,709]. However, a particular highlight of the bond fluctuation model studies was the evidence [493,506,528] that the Gibbs-DiMarzio description of the “entropy catastrophe” at the Kauzmann temperature is an artefact of rather inaccurate approximations. Also attempts to map the lattice model to real polymers gave promising results [329,519]. Finally, also a rather realistic model for the glassy behavior of confined polybutadiene was addressed [1122,1158].

Molecular dynamics simulations were also carried out for two other models of glassforming fluids, the Kob-Anderson binary Lennard-Jones mixture [510,568,684,690,738] and a model for SiO₂ and its mixtures with other oxides [531,535,568,569,597,632,649,672,685] in particular; the logarithmic dependence of the apparent glass transition temperature on the cooling rate [510,535], evidence for the Goetze mode coupling theory [586], evidence for growing dynamic length scales extracted from surface effects [690,738,756,781], and percolative sodium transport in sodium disilicate melts [736] deserve to be mentioned. However, none of these studies gave insight whether or not the structural relaxation time truly diverges at nonzero temperatures, and what a proper “order parameter” distinguishing the glass from the supercooled fluid is. The current state of the art is summarized in a textbook (written with W. Kob) [1035]

6. Studies of macromolecular systems

While a formulation of a Monte Carlo Renormalization Group scheme [121] aimed at a better understanding of the critical exponents describing the self-avoiding walk problem, the first simulation of a dense melt of short chains [128] was motivated by experimental work [130,150] that gave evidence for the Rouse-like motions of the monomers only, not for snakelike “reptation” of the chain in a tube formed by its environment. However, later simulations of much longer chains [307,339,379,418,666] succeeded to study the crossover from the Rouse model to reptation in detail.

A famous problem of polymer science is the adsorption transition of a long flexible macromolecule from a dilute solution (under good solvent conditions) at an attractive wall [149,745,763,1012,1034,1083,1084]. In early work [149], recognizing the analogy to the surface-bulk multicritical point of the phase transitions of semi-infinite n-vector models, the deGennes conjecture for the crossover exponent could be disproven, but the precise value of this exponent has remained controversial for decades, and only recent work [1083] applying the pruned-enriched Rosenbluth method to very long chain molecules and using a comparative study of various ranges of the adsorption potential could clarify the situation. However, open questions still remain concerning the adsorption of semiflexible chains [1084,1182]. The latter show a complicated crossover behavior also in bulk solution, particularly when exposed to stretching forces, which could be elucidated only recently [1039,1052,1077]. The fact that the standard definition of the persistence length of semiflexible polymers holds only for Gaussian “phantom chains” [933] has hampered progress in this field, in particular when the extension to polymers with complex chemical architecture (such as “bottlebrush polymers” [877,904,985,1025,1055]) is considered.

A very interesting problem involving only the statistical mechanics of a single chain concerns confinement inside a tube [188,899,934,1000] or in between parallel plates [455,566,935], or the competition between chain collapse in poor solvents [148,439,969,978] and adsorption [915,945,948,1129]. Related single chain phase transitions (which often show inequivalence between different ensembles of statistical mechanics due to the geometrical constraints that are present) concern the “escape transition” of compressed mushrooms [609,610] or compressed polymers [1107] or the “coil-bridge”-transition [1118]. Polymer collapse in poor solvents gives rise to a rich phase diagram, when bottle-brushes are considered, due to pearl necklace type structures [988,997,1010].

While for phase transition of single chains their connectivity provides unique features, phase transitions in many-chain systems often have analogs in small molecule systems, but show also characteristic differences due to the large size of a polymer coil. Nucleation and spinodal decomposition in polymer mixtures for very long chains behave almost mean-field like [166,169,399]; with respect to the critical point of unmixing, crossover from Ising to mean field behavior is observed with increasing distance from the critical point [390,399,414]. Nevertheless, the Flory-Huggins theory for polymer blends is fairly inaccurate [226], when one extracts Flory-Huggins parameter from scattering experiments via this theory a spurious concentration dependence results [240,264] and the chain linear dimensions depend on the thermodynamic state [251], particularly in semidilute solutions [446]. But early versions of integral equation theories of blends even performed worse [338]. In $d=2$ dimensions, however, the critical temperature scales sublinearly with chain length [744,828]. Particularly interesting is mesophase separation in block copolymer melts [315,318], where simulations revealed a pretransitional stretching (into a dumbbell-like conformation) of the chains, in agreement with experiments performed independently at the same time. Also the interplay of confinement in thin films and lamellar ordering produces a rich phase diagram, relevant for experiment [385,432,622,623], while block copolymers in selective solvent show micelle formation [585,602,654,664,878,930]. These simulations (for finite chain lengths) clearly reveal the shortcomings of the “selfconsistent field theory”, which in theoretical polymer physics often is taken as something like the “gold standard”. Also simulations of “polymer brushes” (chains grafted densely with one chain end on a planar or curved substrate) [336,365,381,434,461,697,750,771,790,837,847,869,906,944,1017,1043,1059,1067,1069,1073,1093,1116,1124] have revealed similar limitations of the standard theories. A problem of great interest both from the point of view of statistical physics and for applications (liquid-crystalline devices, etc) is the occurrence of nematic order in lyotropic solution of semiflexible polymers [1146,1147,1151,1154,1161,1162,1163,1164,1171,1172,1175]. Extensive Molecular Dynamics simulations supplemented with density functional calculations could clarify the shortcomings of some simplified theories. Thus, Monte Carlo simulation for polymeric systems has become a particularly fruitful method.

MITGLIEDSCHAFTEN

- Deutsche Physikalische Gesellschaft
- Hochschulverband
- Institute of Physics, UK (Fellow)
- American Physical Society

Sonderforschungsbereiche der Deutschen Forschungsgemeinschaft

- SFB 130 “Ferroelektrika” 1976 – 1978 Teilprojektleiter
- SFB 125 “Magnetische Momente in Metallen” 1978 - 1983
- SFB 41 “Makromoleküle” 1984 – 1987 Teilprojektleiter
- SFB 262 “Glaszustand und Glasübergang nichtmetallischer

- amorpher Materialien“ 1987 – 2001, Teilprojektleiter
 2002 - 2013 SFB 625 “Von einzelnen Molekülen zu nanoskopisch strukturierten Materialien“
 (Teilprojektleiter 2002-2013)
 2002 - 2013 SFB TR6 “Physik kolloidaler Suspensionen in externen Feldern”
 (Teilprojektleiter 2002-2013)

Organisations- und Programmkomitees von Tagungen

- 1975 NATO Advanced Study Institute, Geilo, Norway
 seit 1975 MECO (Middle European Cooperation on Statistical Physics)
 1979 ICM (International Conference on Magnetism) Munich, Germany
 1979 Jülicher Ferienkurs – The Physics of Alloys, Jülich, Germany
 1980 IUPAP Conference on Statistical Physics, Edmonton, AL / Canada
 1981 Les Houches “Winter School“, Les Houches, France
 1982 Jülicher Ferienkurs – The Physics of Polymers, Jülich, Germany
 1983 IUPAP Conference on Statistical Physics, Edingburgh, Great Britain
 1985 ICM (International Conference on Magnetism) San Francisco, CA, USA
 1986 IUPAP Conference on Statistical Physics, Boston, MA. USA
 1989 IUPAP Conference on Statistical Physics, Rio de Janeiro, Brazil
 1992 IUPAP Conference on Statistical Physics, Berlin, Germany
 1993 13th General Conference of the EPS Condensed Matter Division,
 Regensburg, Germany
 1995 IUPAP Conference on Statistical Physics, Xiamen, China
 1995 Director of Euroconference “Monte Carlo and Molecular
 Dynamics of Condensed Matter Systems” Como, Italy (with G. Ciccotti)
 1996 EPS-APS Conference on Computational Physics, Cracow, Poland
 1998 EPS-APS-IUPAP Conference on Computational Physics, Granada, Spain
 2000 Co-Director of NATO ARW “Multiscale Simulations in Chemistry and Biology”, Eilat,
 Israel (with A. Brandt and J. Bernholc)
 2001 IUPAP Conference on Statistical Physics, Cancun, Mexico
 2001 EPS-APS-IUPAP Conference on Computational Physics, CCP 2001,
 Aachen, Germany (Vice Chairman)
 2002 EPS-APS-IUPAP Conference on Computational Physics, CCP2002, San Diego, USA
 2004 IUPAP Conference on Statistical Physics, Bangalore, India
 2004 EPS-APS-IUPAP Conference on Computational Physics, CCP2004, Genova, Italy
 2005 Co-Director of Erice Summer School, Erice, Italy
 2007 IUPAP Conference on Statistical Physics, Genova, Italy
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 seit 2010 Steering Committee of the Granada Seminar on Computational and Statistical Physics
 2010 IUPAP Conference on Statistical Physics, Cairns, Australia
 2010 EPS-APS-IUPAP Conference on Computational Physics, CCP2010, Trondheim, Norway
 2011 Liquid Matter Conference, Vienna, Austria
 2013 IUPAP “Conference on Statistical Physics”, Seoul, South Korea
 2015 EPS-APS-IUPAP Conference on Computational Physics, CCP 2015, Guwahati, India
 2016 IUPAP Conference on Statistical Physics, Lyon, France
 2020 Liquid Matter Conference, Prague, Czech Republic

MITHERAUSGEBER VON

- 1979 Springer, Berlin *Monte Carlo Methods in Statistical Physics* (2nd Edition 1986)
 1984 Springer, Berlin *Applications of the Monte Carlo Method in Statistical Physics*
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 1992 Springer, Berlin *The Monte Carlo Method in Condensed Matter Physics*

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- 1979 – 1982, 1988 – 1990 Editorial board *Journal of Statistical Physics*
- 1984 – 1989 Editorial board *Journal of Computational Physics*
- 1983 – 2000 Editorial board *Ferroelectrics Letters*
- 1987 – 2007 Editorial board *Computer Physics Communications*
- seit 1991 Editorial board *International Journal of Modern Physics C (Physics and Computers)*
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- 2000 - 2002 Editorial board, *Journal of Statistical Physics*
- 2000 - 2003 Editorial board, *Europhysics Letters*
- 2000 - 2004 Kuratorium, *Physikalische Blätter*
- 2003 - 2005 Editorial board, *Physical Chemistry and Chemical Physics*
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- 2010 – 2012 *Journal of Statistical Physics*
- 2006 - 2011 Editorial board, *Journal of Physics A: Mathematics and General*
- 2011 - 2013 Advisory Board, *Journal of Chemical Physics*

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Ich habe Fachgutachten für die folgenden Institutionen und Trägerschaften erstellt:

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Prof. Dr. Kurt Binder