# Quantum Aspects of Molecular Motions in Solids

Edited by A. Heidemann, A. Magert, M. Prager, D. Richter, and T. Springer



## **Quantum Aspects Of Molecular Motions In Solids**

David P. Landau, K.K. Mon, Heinz-Bernd Schüttler

#### **Quantum Aspects Of Molecular Motions In Solids:**

Quantum Aspects of Molecular Motions in Solids Anton Heidemann, Andreas Magerl, Michael Prager, Dieter Richter, Tasso Springer, 2012-12-06 The Institut Max von Laue Paul Langevin ILL in Grenoble regularly organizes workshops that deal with various applications of neutrons in physics chemistry biology and materials science The workshop Quantum Aspects of Molecular Motions in Solids was jointly organized by the Institut Laue Langevin and the Institut für Festkorperforschung at the Kernforschungsan lage Jiilich and took place in September 1986 in Grenoble Tunneling phenomena in molecular crystals were first observed with macro scopic methods like specific heat experiments and later also with NMR Fi nally the development of high resolution neutron scattering techniques like neutron backscattering led to direct spectroscopic observation of the tunnel split ground state This breakthrough was achieved in 1975 at Jiilich Since then the large variety of high resolution techniques available in combination with high neutron flux have turned ILL into the leading laboratory in the field of tunneling spectroscopy Since 1980 regular meetings of scientists involved in this topic have been organized every two years Jiilich Braunschweig Nottingham and have led to an intense exchange of ideas and experimental results The present workshop is the fourth of this series and the first with published proceedings presenting the state of the art in this field The eight review articles introduce scientists not involved in the subject to the actual discussion Sessions on translational tunneling of light interstitials in metals as well as on tunneling phenomena in amorphous substances provide bridges to adjacent fields Quantum Aspects of Molecular Motions in Solids Anton Heidemann, Andreas Magerl, Michael Quantum Aspects of Molecular Motions in Solids ,1987 Prager, 1987-03-05 Workshop on Quantum Aspects of Molecular Motions in Solids, September 24-26, 1986, 1986 **Computer Simulation Studies in Condensed-Matter** Physics XIII D.P. Landau, S.P. Lewis, H.-B. Schüttler, 2012-12-06 Almost fifteen years ago because of the phenomenal growth in the power of computer simulations The University of Georgia formed the first institutional unit devoted to the use of simulations in research and teaching The Center for Simulational Physics As the international simulations community expanded further we sensed a need for a meeting place for both experi enced simulators and neophytes to discuss new techniques and recent results in an environment which promoted extended discussion As a consequence the Center for Simulational Physics established an annual workshop on Re cent Developments in Computer Simulation Studies in Condensed Matter Physics This year s workshop was the thirteenth in this series and the con tinued interest shown by the scientific community demonstrates quite clearly the useful purpose that these meetings have served The latest workshop was held at The University of Georgia February 21 25 2000 and these proceed ings provide a status report on a number of important topics This volume is published with the goal of timely dissemination of the material to a wider audience We wish to offer a special thanks to the IBM Corporation for its generous support of this year's workshop We also acknowledge the Donors of the Petroleum Research Fund administered by the American Chemical Society and the National Science

Foundation for partial support This volume contains both invited papers and contributed presentations on problems in both classical and quantum condensed matter physics 

Computer Simulation Studies in Condensed-Matter Physics VIII David P. Landau, Kin-Keung Mon, Heinz-Bernd Schüttler, 2012-12-06 Computer Simulation Studies in Condensed Matter Physics VIII covers recent developments in this field presented at the 1995 workshop such as new algorithms methods of analysis and conceptual developments This volume is composed of three parts The first part contains invited papers that deal with simulational studies of classical systems The second part is devoted to invited papers on quantum systems including new results for strongly correlated electron and quantum spin models The final part comprises contributed presentations

Computer Simulation Studies in Condensed-Matter Physics IV David P. Landau, K.K. Mon, Heinz-Bernd Schüttler, 2012-12-06 The contribution of computer simulation studies to our understanding of proper ties of a wide range of condensed matter systems is now well established The Center for Simulational Physics has been hosting annual workshops with the in tent of bringing together some of the experienced practitioners in the field as well as relative newcomers in the field to provide a forum for the exchange of ideas and recent results This year s workshop the fourth in the series was held at the University of Georgia February 18 22 1991 These proceedings are a record of the workshop and are published with the goal of timely dissemination of the papers to a wider audience The proceedings are divided into three parts The first part contains invited papers which deal with simulational studies of classical systems and includes an introduction to some new simulation techniques and special purpose comput ers as well A separate section of the proceedings is devoted to invited papers on quantum systems including new results for strongly correlated electron and quantum spin models believed to be important for the description of high T c superconductors The contributed presentations comprise the final chapter

Computer Simulation Studies in Condensed-Matter Physics XI David P. Landau, Heinz-Bernd Schüttler, 2012-12-06 More than a decade ago because of the phenomenal growth in the power of computer simulations. The University of Georgia formed the first institutional unit devoted to the use of simulations in research and teaching. The Center for Simulational Physics As the simulations community expanded further we sensed a need for a meeting place for both experienced simulators and neophytes to discuss new techniques and recent results in an environment which promoted extended discussion As a consequence the Center for Simulational Physics established an annual workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics This year's workshop was the eleventh in this series and the interest shown by the scientific community demonstrates quite clearly the useful purpose which the series has served The latest workshop was held at The University of Georgia February 23 27 1998 and these proceedings provide a status report on a number of important topics. This volume is published with the goal of timely dissemination of the material to a wider audience. We wish to offer a special thanks to IBM Corporation for their generous support of this year's workshop. This volume contains both invited papers and contributed presentations on problems in both classical and quantum condensed.

matter physics We hope that each reader will benefit from specialized results as well as profit from exposure to new algorithms methods of analysis and conceptual developments Athens GA U S A D P Landau April 1998 H B Simulation Studies in Condensed-Matter Physics XII D. P. Landau, S. P. Lewis, H.-B. Schüttler, 2012-12-06 More than a decade ago because of the phenomenal growth in the power of computer simulations The University of Georgia formed the first institutional unit devoted to the use of simulations in research and teaching The Center for Simulational Physics As the simulations community expanded further we sensed a need for a meeting place for both experienced simulators and neophytes to discuss new techniques and recent results in an environment which promoted extended discussion As a consequence the Center for Sim ulational Physics established an annual workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics This year's workshop was the twelfth in this series It was held at The University of Geor gia March 8 12 1999 as an unofficial satellite conference to the Centennial Meeting of the American Physical Society in Atlanta GA The continued interest shown by the scientific community demonstrates quite clearly the useful purpose which the series has served These proceedings provide a sta tus report on a number of important topics This volume is published with the goal of timely dissemination of the material to a wider audience We wish to offer special thanks to IBM Corporation for their generous support of this year s workshop This volume contains both invited papers and contributed presentations on problems in both classical and quantum condensed matter physics. We hope that each reader will benefit from specialized results as well as profit from exposure to new algorithms methods of analysis and conceptual Computer Simulation Studies in Condensed-Matter Physics VI David P. Landau, K.K. devel opments Mon, Heinz-Bernd Schüttler, 2012-12-06 Computer Simulation Studies in Condensed Matter Physics VI provides a broad overview of recent developments in this field Based on the last workshop it presents invited and contributed papers which describe new physical results simulational techniques and ways of interpreting simulational data Both classical and quantum systems are discussed Computer Simulation Studies in Condensed-Matter Physics IX David P. Landau, Kin-Keung Mon, Heinz-Bernd Schüttler, 2012-12-06 Computer Simulation Studies in Condensed Matter Physics IX covers recent developments in this field This workshop was the ninth in this series and was held at the University of Georgia March 49 1996 and these proceedings form a record which is published with the goal of timely dissemination of the material to a wider audience This volume is composed of three parts The first section contains invited papers that deal with simulational studies of classical systems The second section of the proceedings is devoted to invited papers on quantum systems including new results for strongly correlated electron and quantum spin models. The final section comprises contributed presentations

The Structure and Conformation of Amphiphilic Membranes Reinhard Lipowsky, Dieter Richter, Kurt Kremer, 2013-03-08 Membranes composed of amphiphilic molecules are highly flexible surfaces that determine the architecture of biological systems and provide a basic structural element for complex fluids such as microemulsions Recently

a variety of new experimental methods such as X ray scattering neutron scattering and atomic force microscopy have been used in order to study themolecular structure of these membranes Their conformational behavior on the other hand is studied by optical and electron microscopy which reveals that membranes in aqueous solution exhibit an amazing variety of different shapes Several theoretical concepts are described suchas bending elasticity curvature and minimal surfaces in order to understand this polymorphism These concepts are also useful to describe the behavior of membranes in complex fluids where they can build up hexagonal lamellar triply periodic cubic and sponge phases The contributions to this volume provide an up to date overview and describe the state of the art of this rapidly evolving field of research **Domain in Surface and Structural Dynamics** G.J Long, F. Grandjean, 2012-12-06 About two years ago while studying the dynamic properties of Fe CO II we realized that there 3 was virtually no single source of infonnation on the structural dynamics of materials. The time domain of different dynamic structural processes covers many orders of magnitude and may be in vestigated by numerous vastly different experimental techniques Indeed the subject seemed ap propriate for a NATO Advanced Study Institute at which we could bring together chemists physicists metallurgists and bioscientists using the various techniques for the study of sundry time sensitive materials The actual Advanced Study Institute which met in II Ciocco Italy from 14 to 26 June 1987 was in fact a dynamic experience for those of us involved Now we have come to the final phase the communication of the results of this Advanced Study Institute to the general scientific community In so doing we hope to provide in one place a convenient source of infor mation on dynamics at the surface and within a solid state material The beautiful mountainous setting of Tuscany and especially the idyllic surroundings of II Ciocco provided an ideal venue for the Advanced Study Institute Our field trip to Pisa linked our topic to the history of time measurement through a visit to the Pisa cathedral where presumably Galileo first conceived the isochronism of the simple pendulum and its use in time Computer Simulation Studies in Condensed-Matter Physics VII David P. Landau, K.K. measurement Mon, Heinz-Bernd Schüttler, 2012-12-06 Computer Simulation Studies in Condensed Matter Physics VII provides a broad overview of recent developments Presented at the recent workshop it contains the invited and contributed papers which describe new physical results simulational techniques and ways of interpreting simulational data Both classical and quantum Exotic Atoms in Condensed Matter Giorgio Benedek, Hubert Schneuwly, 2012-12-06 Exotic Atoms systems are discussed in Condensed Matter reviews the state of the art in this field from meson factories to the basic interactions of muons in condensed matter The application of muon and pion based analysis of solid state structural magnetic and superconducting properties is discussed The spectroscopic features of exotic atoms are reviewed together with their application to chemical analysis Also muon catalyzed fusion is presented Surface Science Russel F. Howe, Robert N. Lamb, Klaus Wandelt, 2013-03-07 Surface science has existed as a recognized discipline for more than 20 years During this period the subject has expanded in two important ways On the one hand the techniques available for studying surfaces both

experimental and theoretical have grown in number and in sophistication On the other hand surface science has been applied to an increasing number of areas of technology such as catalysis semicon ductor processing new materials development corrosion prevention adhesion and tribology There is however no sharp division between fundamental and applied surface science New techniques can immediately be applied to technologically important problems Improvements in understanding of fundamental phenomena such as epi taxial growth of one metal on another or the bonding of hydrocarbons to metal sur faces to name just two examples have direct consequences for technology Surface science has also become very much an interdisciplinary subject physics chemistry materials science chemical and electronical engineering all draw upon and contribute to surface science The intimate relationship between principles and applications of surface science forms the theme of this proceedings volume The contributions were all presented as invited lectures at an Australian German Workshop on Surface Science held at Coogee Beach Sydney Australia in December 1991 The contributors all active surface scientists in their respective countries were asked to highlight recent develop ments in their own areas of activity involving new techniques advances in funda mental understanding or new applications in technology Computational Approaches in Condensed-Matter Physics Seiji Miyashita, Masatoshi Imada, Hajime Takayama, 2012-12-06 Interacting many body systems are the main subjects of research in theoretical condensed matter physics and they are the source of both the interest and the difficulty in this field In order to understand the macroscopic properties of matter in terms of macroscopic knowledge many analytic and approximate methods have been introduced The contributions to this proceedings volume focus on the most recent developments of computational approaches in condensed matter physics Monte Carlo methods and molecular dynamics simulations applied to strongly correlated classical and quantum systems such as electron systems quantum spin systems spin glassss coupled map systems polymers and other random and comlex systems are reviewed Comprising easy to follow introductions to each field covered and also more specialized contributions this proceedings volume explains why computational approaches are necessary and how different fields are related to each other Photons and Continuum States of Atoms and Molecules Carla Guidotti, Maria Allegrini, 2012-12-06 Since 1981 there has been an attempt in Europe to organize a series of small meetings workshops tavole rotonde with the aim of bringing together physi cists and chemists interested in problems concerning atoms or molecules in teracting with external photons where the continua are investigated The number of problems that fall into this category turns out to be vast However it is not possible to make a strict separation into problems con cerning atomic and molecular collisions and those related to the usual spec troscopy This admixture of two disciplines discussions on the role of photons and on the interaction of external electromagnetic fields with the continuum provided a central motivation for these workshops The fourth of this series of meetings was held at Cortona between June 16 and 20 1986 It was attended by about 100 researchers in the field and there were 43 presentations all having equal time These talks form the subject matter of this volume The idea of publishing the proceedings of these meetings is not new It

allows one to have small meetings in which the subject matter can be discussed at length in a lively atmosphere However after the meeting is over the speakers can collect their thoughts and produce articles in which the results of their interaction with the other participants can be incorporated Computer Simulation Studies in Condensed-Matter Physics V David P. Landau, K.K. Mon, Heinz-Bernd Schüttler, 2012-12-06 As the role of computer simulations began to increase in importance we sensed a need for a meeting place for both experienced simulators and neophytes to discuss new techniques and results in an evironment which promotes extended discussion As a consequence of these concerns The Center for Simulational Physics established an annual workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics This year s workshop was the fifth in this series and the interest which the scientific community has shown demonstrates quite clearly the useful purpose which the series has served The workshop was held at the University of Georgia February 17 21 1992 and these proceedings form a record of the workshop which is published with the goal of timely dissemination of the papers to a wider audience The proceedings are divided into four parts The first part contains invited papers which deal with simulational studies of classical systems and includes an introduction to some new simulation techniques and special purpose computers as well A separate section of the proceedings is devoted to invited papers on quantum systems including new results for strongly correlated electron and quan tum spin models. The third section is comprised of a single invited description of a newly developed software shell designed for running parallel programs The contributed presentations Computer Simulation Studies in Condensed-Matter Physics X David P. Landau, Kin-Keung comprise the final chapter Mon, Heinz-Bernd Schüttler, 2012-12-06 Computer Simulation Studies in Condensed Matter Physics X is devoted to Prof Masuo Suzuki s ideas which have made novel new simulations possible These proceedings of the 1997 workshop comprise three parts that deal with new algorithms methods of analysis and conceptual developments The first part contains invited papers that deal with simulational studies of classical systems The second of the proceedings is devoted to invited papers on quantum systems including new results for strongly correlated electron and quantum spin models. The final part contains a large number of contributed presentations

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