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V.L.Broude E.I. Rashba E.F. Sheka

Spectroscopy of Molecular Excitons



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# **Spectroscopy Of Molecular Excitons**

**Chern Chuang** 

## **Spectroscopy Of Molecular Excitons:**

Spectroscopy of Molecular Excitons Vladimir L. Broude, Emmanuel I. Rashba, Elena F. Sheka, 1985 Low temperature spectroscopy of organic molecular crystals came into being in the late 20s just when quantum physics of solids as a whole began to de velop vigorously Already in the early works two experimental facts of prime importance were discovered the presence of a multitude of narrow bands in the low temperature spectrum of a crystal and a close relationship between the spectrum of the crystal and that of the constituent molecules These findings immediately preceded the celebrated paper of Frenkel in which he went beyond the framework of Bloch's scheme and advanced the exciton concept Subsequent investigations showed that the most interesting features of the spectra of molecular crystals are associated with excitons and then the spectroscopy of molecular excitons began to form gradually on the basis of the spectroscopy of organic crystals The molecular exciton became synonymous to the Frenkel exciton in a molecular crystal In view of the difficulties involved in the analysis of rich spectra con taining many tens of bands the spectroscopy of molecular crystals had long been connected most closely with the spectroscopy of molecules It had deve loped independently to a large extent from the other branches of solid state physics This was also emphasized by the difference in experimental techniques the specific properties of the objects etc As a result there was some lag in ideas and concepts Spectroscopy of Molecular Excitons Vladimir L. Broude, Emmanuel I. Rashba, Elena F. Sheka, 1985-09-01 Low temperature spectroscopy of organic molecular crystals came into being in the late 20s just when quantum physics of solids as a whole began to de velop vigorously Already in the early works two experimental facts of prime importance were discovered the presence of a multitude of narrow bands in the low temperature spectrum of a crystal and a close relationship between the spectrum of the crystal and that of the constituent molecules These findings immediately preceded the celebrated paper of Frenkel in which he went beyond the framework of Bloch's scheme and advanced the exciton concept Subsequent investigations showed that the most interesting features of the spectra of molecular crystals are associated with excitons and then the spectroscopy of molecular excitons began to form gradually on the basis of the spectroscopy of organic crystals The molecular exciton became synonymous to the Frenkel exciton in a molecular crystal In view of the difficulties involved in the analysis of rich spectra con taining many tens of bands the spectroscopy of molecular crystals had long been connected most closely with the spectroscopy of molecules It had deve loped independently to a large extent from the other branches of solid state physics This was also emphasized by the difference in experimental techniques the specific properties of the objects etc As a result there was some lag in ideas and Spectroscopy of Molecular Excitons Vladimir L'vovich Broude, Émmanuil Iosifovich Rashba, Elena Fedorovna concepts Sheka,1985 Photosynthetic Excitons Herbert van Amerongen, Leonas Valk?nas, Rienk van Grondelle, 2000 Excitons are considered as the basic concept used by describing the spectral properties of photosynthetic pigment protein complexes and excitation dynamics in photosynthetic light harvesting antenna and reaction centers Following the recently obtained

structures of a variety of photosynthetic pigment protein complexes from plants and bacteria our interest in understanding the relation between structure function and spectroscopy has strongly increased These data demonstrate a short interpigment distance of the order of 1 nm or even smaller and or a highly symmetric ring like arrangement of pigment molecules in peripheral light harvesting complexes of photosynthetic bacteria Books which were devoted to the exciton problem so far mainly considered the spectral properties of molecular crystals However the small size of these pigment aggregates in the pigment protein complexes as well as the role of the protein which is responsible for the structural arrangement of the complex clearly will have a dramatic influence on the pigment spectra and exciton dynamics All these aspects of the problem are considered in this book Exciton theory is mainly considered for small molecular aggregates dimers ring like structures etc Together with the theoretical description of the classical conceptual approach which mainly deals with polarization properties of the absorption and fluorescence spectra the nonlinear femtosecond spectroscopy which is widely used for investigations now is also discussed A large part of the book demonstrates the excitonic effects in a multitude of photosynthetic pigment protein complexes and how we can understand these properties on the basis of the **Dynamics of Molecular Excitons** Seogjoo J. Jang, 2020-04-29 Dynamics of Molecular Excitons provides exciton concept a comprehensive but concise description of major theories on the dynamics of molecular excitons intended to serve as a self contained resource on the topic Designed to help those new to this area gain proficiency in this field experts will also find the book useful in developing a deeper understanding of the subject The starting point of the book is the standard microscopic definition of molecular Hamiltonians presented in commonly accepted modern quantum mechanical notations Major assumptions and approximations involved in constructing Frenkel type exciton Hamiltonians which are well established but are often hidden under arcane notations and approximations of old publications are presented in detail This will help quantum chemists understand the major assumptions involved in the definition of commonly used exciton models Rate theories of exciton dynamics such as F rster and Dexter theories and their modern generalizations are presented in a unified and detailed manner In addition important aspects that are often neglected such as local field effect and the role of fluctuating environments are discussed Various quantum dynamics methods allowing coherent dynamics of excitons are presented in a systematic manner in the context of quantum master equations or path integral formalisms. The author also provides a detailed theoretical explanation for the major spectroscopic techniques probing exciton dynamics including modern two dimensional electronic spectroscopy with a critical assessment of the implications of these spectroscopic measurements Finally the book includes a brief overview of major applications including an explanation of organic photovoltaic materials and natural light harvesting complexes Molecular Spectroscopy—XI O. Sild,2017-01-31 Molecular Spectroscopy XI provides information pertinent to the fundamental aspects of molecular spectroscopy This book discusses the modifications of molecular spectra when the density varies as a function of temperature and pressure

Organized into 15 chapters this book begins with an overview of the several processes concerning triplet excitons leading to magnetic field sensitive luminescence in organic crystals and related compounds This text then examines the methods of investigation of the exciton band structures in molecular crystals Other chapters consider the conditions for the equivalence of Fourier spectroscopy and of slow passage experiments in nuclear magnetic resonance This book discusses as well the application of computer technology in carbon 13 magnetic resonance spectroscopy The final chapter deals with the application of high resolution proton and carbon 13 n m r spectroscopy for the investigation of the molecular conformations in proteins This book is a valuable resource for organic chemists biologists microbiologists scientists and research workers

Spectroscopy of the Excited State Baldassare Di Bartolo, 2012-12-06 These proceedings report the lectures and seminars presented at the NATO Advanced Study Institute on The Spectroscopy of the Excited State held at Erice Italy June 9 24 1975 This Institute was an activity of the International School of Atomic and Molecular Spectroscopy of the Ettore Majorana Centre for Scientific Culture The Institute consisted of a series of lectures on the spectroscopic properties of materials in excited electronic states that starting at a fundamental level finally reached the current level of research The sequence of lectures and the organization of the material taught were in keeping with a didac tical presentation. In essence the course had the two fold pur pose of organizing what was known on the subject and updating the knowledge in the field The formal lectures were complemented by seminars whose abstracts are also included in these proceedings. The proceedings report also the contributions sent by Professors R G W Norrish and S C1aesson who unfortunately were not able to come because of illness A total of 62 participants and 7 lecturers came from the following countries Belgium Canada Czechoslovakia France Germany Israel Italy Japan Netherlands Norway Pakistan Poland Sweden Switzerland the United Kingdom the United States and Venezuela The secretaries of the course were A La Francesca for the administrative aspects of the meeting and P Papagiannakopou10s for the scientific aspects of the meeting Two-dimensional Spectroscopy of Molecular Excitons in a Model Dimer System H. Alexei Halpin, 2014 **Theory of Molecular Excitons** A. Davydov, 2013-11-11 Spectroscopy, Relaxation, and Transport of Molecular Excitons in Noisy and Disordered Environments Chern Chuang, 2018 In this thesis contribution we theoretically investigate the spectroscopy relaxation and transport properties of Frenkel excitons in molecular aggregates with extensive comparison to or prediction of experimental observables Particular emphasis is devoted to the effects of thermal noise static disorder and system dimensionality Our key contributions are summarized as the following We study the spectroscopic signatures of excitonic molecular aggregates of dimensionality larger than unity as functions of temperature and disorder strength These findings are applied to the determination of essential system characteristics and quantitatively explain the spectroscopic traits seen in experiments where either the temperature or disorder strength is altered A classification scheme generalized from Kasha's seminal work on J and H aggregates is proposed that is compatible with experimental observations previously unexplained We recognize the importance of long

wavelength approximations in understanding the density of states in two dimensional excitonic aggregates And for tubular aggregates this leads to a simple expression for the energy gap between the parallel and the perpendicular polarized peaks useful in inferring key system parameters This long wavelength approach is then extended to the analysis of 2D excitonic molecular aggregates in general A universal scaling relation concerning the steady state diffusive transport of excitons in molecular tubes is predicted and analyzed where the key order parameter is identified as the ratio between the localization length of the exciton wavefunctions and the tube circumference A unified theoretical framework is proposed to explain the relaxation of hot excitons generated in emissive conjugated polymers across three orders of magnitude in timescale with quantitative agreements with experiments **Bose-Einstein Condensation of Excitons and Biexcitons** Svi altoslav Anatol'evich Moskalenko, D. W. Snoke, 2000-02-28 Bose Einstein condensation of excitons is a unique effect in which the electronic states of a solid can self organize to acquire quantum phase coherence The phenomenon is closely linked to Bose Einstein condensation in other systems such as liquid helium and laser cooled atomic gases. This is the first book to provide a comprehensive survey of this field covering theoretical aspects as well as recent experimental work After setting out the relevant basic physics of excitons the authors discuss exciton phonon interactions as well as the behaviour of biexcitons They cover exciton phase transitions and give particular attention to nonlinear optical effects including the optical Stark effect and chaos in excitonic systems. The thermodynamics of equilibrium quasi equilibrium and nonequilibrium systems are examined in detail The authors interweave theoretical and experimental results throughout the book and it will be of great interest to graduate students and researchers in semiconductor and superconductor physics quantum optics and atomic physics

Crystal Optics with Spatial Dispersion, and Excitons Vladimir M. Agranovich, V. Ginzburg, 2013-06-29 Spatial dispersion namely the dependence of the dielectric constant tensor on the wave vector i e on the wavelength at a fixed frequency is receiving increased attention in electrodynamics and condensed matter optics partic ularly in crystal optics In contrast to frequency dispersion namely the frequency dependence of the dielectric constant spatial dispersion is of interest in optics mainly when it leads to qualitatively new phenomena One such phenomenon has been well known for many years it is the natural optical activity gyrotropy But there are other interesting effects due to spatial dispersion namely new normal waves near absorption lines optical anisotropy of cubic crystals and many others Crystal optics that takes spatial dispersion into account includes classical crystal optics with frequency dispersion only as a special case In our opinion this fact alone justifies efforts to develop crystal optics with spatial dispersion taken into account although admittedly its influence is smaH in some cases and it is observable only under rather special conditions Furthermore spatial dispersion in crystal optics deserves attention from another point as well namely the investigation of excitons that can be excited by light We contend that crystal optics with spatial dispersion and the theory of excitons are fields that overlap to a great extent and that it is sometimes quite impossible to separate them It is our aim to show the true interplay be tween these interrelations and to

combine the macroscopic and microscopic approaches to crystal optics with spatial dispersion and exciton theory

Molecular Spectroscopy Yukihiro Ozaki, Marek Januz Wójcik, Jürgen Popp, 2019-04-26 Uniquely creates a strong bridge between molecular spectroscopy and quantum chemistry This two volume book consists of many reviews reporting new applications of quantum chemistry to molecular spectroscopy Raman infrared near infrared terahertz far ultraviolet etc It contains brief introductions to quantum chemistry for spectroscopists and to the recent progress on molecular spectroscopy for quantum chemists Molecular Spectroscopy A Quantum Chemistry Approach examines the recent progress made in the field of molecular spectroscopy the state of the art of quantum chemistry for molecular spectroscopy and more It offers multiple chapters covering the application of quantum chemistry to visible absorption and fluorescence Raman spectroscopy infrared spectroscopy near infrared spectroscopy terahertz spectroscopy and far ultraviolet spectroscopy It presents readers with hydrogen bonding studies by vibrational spectroscopy and quantum chemistry as well as vibrational spectroscopy and quantum chemistry studies on both biological systems and nano science The book also looks at vibrational anharmonicity and overtones and nonlinear and time resolved spectroscopy Comprehensively covers existing and recent applications of quantum chemistry to molecular spectroscopy Introduces the quantum chemistry for the field of spectroscopy and the advancements being made on molecular spectroscopy for quantum chemistry Edited by world leading experts who have long standing extensive experience and international standing in the field Molecular Spectroscopy A Quantum Chemistry Approach is an ideal book for analytical chemists theoretical chemists chemists biochemists materials scientists biologists and physicists Advances in Multi-Photon Processes and Spectroscopy S. H. Lin, A. A. Villaeys, 2004 In view of interested in the subject the rapid growth in both experimental and theoretical studies of multiphoton processes and multiphoton spectroscopy of atoms ions and molecules in chemistry physics biology material sciences etc it is desirable to publish an Advanced Series that contains review papers readable not only by active researchers in these areas but also by those who are not experts in the field but who intend to enter the field The present series attempts to serve this purpose Each review article is written in a self contained manner by the experts in the area so that the readers can grasp the knowledge in the area without too much preparation The topics covered in this volume include OC Ultrafast Photochemical Dynamics in Solution Studied by Femtosecond Time Resolved Fluorescence Spectroscopy Involvement of Highly Excited StatesOCO OC Spectral Selective Studies of Molecular Doped Solids and ApplicationsOCO OC From Multiphoton to Tunnel IonizationOCO OC Cluster Dynamics in Intense Laser FieldsOCO and OC Molecular Theory of Sum Frequency Generation and its Application to Study Molecular ChiralityOCO It is hoped that the collection of topics in this volume will be useful not only to active researchers but also to other scientists in biology chemistry materials science and physics This book has been selected for coverage in OCo CC Physical Chemical Spectral Selective Studies of Molecular Doped Solids and Applications J P Galaup From Multiphoton to Tunnel Ionization S L Chin Cluster Dynamics in Intense Laser Fields D Mathur Molecular Theory of Sum

frequency Generations and Its Applications to Study Molecular Chirality M Hayashi S H Lin Readership Graduate students and researchers in chemistry biology materials science and physics Advances In Multi-photon Processes And Spectroscopy, Vol 16 Sheng-hsien Lin, Albert A Villaeys, Yuichi Fujimura, 2004-09-09 In view of the rapid growth in both experimental and theoretical studies of multiphoton processes and multiphoton spectroscopy of atoms ions and molecules in chemistry physics biology material sciences etc it is desirable to publish an Advanced Series that contains review papers readable not only by active researchers in these areas but also by those who are not experts in the field but who intend to enter the field The present series attempts to serve this purpose Each review article is written in a self contained manner by the experts in the area so that the readers can grasp the knowledge in the area without too much preparation The topics covered in this volume include Ultrafast Photochemical Dynamics in Solution Studied by Femtosecond Time Resolved Fluorescence Spectroscopy Involvement of Highly Excited States Spectral Selective Studies of Molecular Doped Solids and Applications From Multiphoton to Tunnel Ionization Cluster Dynamics in Intense Laser Fields and Molecular Theory of Sum Frequency Generation and its Application to Study Molecular Chirality It is hoped that the collection of topics in this volume will be useful not only to active researchers but also to other scientists in biology chemistry materials science and physics This book has been selected for coverage in CC Physical Chemical Earth Sciences Index to Scientific Book Contents ISBC

**Electronic Excitations in Organic Based Nanostructures** ,2003-11-13 The first book devoted to a systematic consideration of electronic excitations and electronic energy transfer in organic crystalline multilayers and organics based nanostructures quantum wells quantum wires quantum dots microcavities. The ingenious combination of organic with inorganic materials in one and the same hybrid structure is shown to give qualitatively new opto electronic phenomena potentially important for applications in nonlinear optics light emitting devices photovoltaic cells lasers and so on The book will be useful not only for physicists but also for chemists and biologists To help the nonspecialist reader three Chapters which contain a tutorial and updated introduction to the physics of electronic excitations in organic and inorganic solids have been included hybrid Frenkel Wannier Mott excitons microcavities with crystalline and disordered organics electronic excitation at donor acceptor interfaces cold photoconductivity at donor acceptor interface cummulative photovoltage Feorster transfer energy in microcavity New concepts for LEDs **Optical Properties of Mixed Crystals** R.J. Elliott, I.P. Ipatova, 2012-12-02 Optical Properties of Mixed Crystals is concerned with the description of optical processes in substitutionally disordered semiconductors and insulators which can be basically described through their elementary excitations Two of the chapters relate to the phonon response including the effect of side bands on electron transitions Two relate to electronic spectra one on photoelectron spectroscopy and the other on excitons A further chapter deals with magnons in magnetic crystals and a final chapter is related to fluctuations and band edge effects Each chapter deals with a specific class of excitation but the book makes it clear that the fundamental structure of the excitation spectra including band formation band tailing and localisation is common to every type of excitation The volume shows how some basic concepts and ideas can be widely applied to bring coherence and understanding to a diverse area of solid state physics. It therefore provides an up to date summary of the experimental and theoretical situation in an important and rapidly developing field and brings together for the first time a discussion of the many different types of spectra which appear in mixed crystals

Materials for Sustainable Energy Vincent Dusastre, 2011 The search for cleaner cheaper smaller and more efficient energy technologies has to a large extent been motivated by the development of new materials. The aim of this collection of articles is therefore to focus on what materials based solutions can offer and show how the rationale design and improvement of their physical and chemical properties can lead to energy production alternatives that have the potential to compete with existing technologies In terms of alternative means to generate electricity that utilize renewable energy sources the most dramatic breakthroughs for both mobile i e transportation and stationary applications are taking place in the fields of solar and fuel cells And from an energy storage perspective exciting developments can be seen emerging from the fields of rechargeable batteries and hydrogen storage Excitonic Processes in Solids Masayasu Ueta, Hiroshi Kanzaki, Koichi Kobayashi, Yutaka Toyozawa, Eiichi Hanamura, 2012-12-06 An exciton is an electronic excitation wave consisting of an electron hole pair which propagates in a nonmetallic solid Since the pioneering research of Fren kel Wannier and the Pohl group in the 1930s a large number of experimental and theoretical studies have been made Due to these investigations the exciton is now a well established concept and the electronic structure has been clarified in great detail The next subjects for investigation are naturally dynamical processes of excitons such as excitation relaxation annihilation and molecule formation and in fact many interesting phenomena have been disclosed by recent works These excitonic processes have been recognized to be quite important in solid state physics because they involve a number of basic interactions between excitons and other elementary excitations It is the aim of this quasi monograph to describe these excitonic processes from both theoretical and experimental points of view we take a few To discuss and illustrate the excitonic processes in solids important and well investigated insulating crystals as playgrounds for excitons on which they play in a manner characteristic of each material The selection of the materials is made in such a way that they possess some unique properties of excitonic processes and are adequate to cover important interactions in which excitons are involved In each material excitonic processes are described in detail from the experimental side in order to show the whole story of excitons in a particular material

**Optical Properties Of Low-dimensional Materials** Yoshihiko Kanemitsu, Tetsuo Ogawa, 1996-01-18 This book surveys recent experimental and theoretical studies on optical properties of low dimensional materials e.g. artificial crystals in zeolites C60 and its related compounds silicon nanostructures including porous Si II VI and III V semiconductor quantum structures and Pb based natural quantum well systems The eight excellent detailed review articles are written by authorities on each field in Japan All the materials introduced in this book yield new optical phenomena originating from their

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