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Electronic Structure and Transport Properties of Bi_2Te_3 and Bi_2Se_3 Single Crystals

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Abstract: The electrical resistivity and the Hall effect of topological insulator Bi_2Te_3 and Bi_2Se_3 single crystals were studied in the temperature range from 4.2 to 300 K and in magnetic fields up to 10 T. Theoretical calculations of the electronic structure of these compounds were carried out in density functional approach, taking into account spin–orbit coupling and crystal structure data for temperatures of 5, 50 and 300 K. A clear correlation was found between the density of electronic states at the Fermi level and the current carrier concentration. In the case of Bi_2Te_3, the density of states at the Fermi level and the current carrier concentration increase with increasing temperature, from 0.296 states eV^{-1} $cell^{-1}$ (5 K) to 0.307 states eV^{-1} $cell^{-1}$ (300 K) and from 0.9×10^{19} cm^{-3} (5 K) to 2.6×10^{19} cm^{-3} (300 K), respectively. On the contrary, in the case of Bi_2Se_3, the density of states decreases with increasing temperature, from 0.201 states eV^{-1} $cell^{-1}$ (5 K) to 0.198 states eV^{-1} $cell^{-1}$ (300 K), and, as a consequence, the charge carrier concentration also decreases from 2.94×10^{19} cm^{-3} (5 K) to 2.81×10^{19} cm^{-3} (300 K).

Keywords: 2D materials; topological insulator; Bi_2Te_3; Bi_2Se_3; electronic structure; DFT; materials informatics; topological resistivity; Hall effect; current carrier concentration

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1. Introduction

The quantum Hall effect, in which the Hall conductivity of a two-dimensional insulator in a high magnetic field is quantized, is one of the important discoveries in condensed matter physics [1]. Special conducting edge states appear in the material in the quantum Hall effect regime. This effect is shown to have a topological nature, and such edge states can be associated with a topological invariant called the Chern number [2,3]. A nonzero Chern number determines the presence of conducting edge states, and a zero Chern number means an insulating state in the bulk, which is observed in the quantum Hall effect. Thus, topological materials can be considered as a special state of matter at the intersection of real materials and abstract mathematical topology. Such materials include topological insulators and topological semimetals. The quantum Hall effect can be considered the first two-dimensional topological insulator. Then, three-dimensional topological insulators were theoretically predicted [4,5] and experimentally discovered [6,7]. Recently, Dirac and Weyl topological semimetals were discovered [8–12].

A topological insulator is an insulator or semiconductor in bulk, whereas a special quantum state of electrons occurs on its surface, which makes charge carriers "topologically protected" from scattering. Such surface states are analogues of the edge states in the quantum Hall effect, and the spin–orbit coupling plays a role of the magnetic field. The metallic surface states of a topological insulator are called Dirac cones, which can be

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Kathleen Armour

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Electronic Structure and Transport Properties of Crystals William F. Leonard,Thomas Lyle Martin,1980 Physics and Chemistry of Finite Systems: From Clusters to Crystals Peru Jena,S.N. Khanna,B.K.N. Rao,2013-11-11 Recent innovations in experimental techniques such as molecular and cluster beam epitaxy supersonic jet expansion matrix isolation and chemical synthesis are increasingly enabling researchers to produce materials by design and with atomic dimension These materials constrained by sire shape and symmetry range from clusters containing as few as two atoms to nanoscale materials consisting of thousands of atoms They possess unique structuraI electronic magnetic and optical properties that depend strongly on their size and geometry The availability of these materials raises many fundamental questions as weIl as technological possibilities From the academic viewpoint the most pertinent question concerns the evolution of the atomic and electronic structure of the system as it grows from micro clusters to crystals At what stage for example does the cluster look as if it is a fragment of the corresponding crystal How do electrons forming bonds in micro clusters transform to bands in solids How do the size dependent properties change from discrete quantum conditions as in clusters to boundary constrained bulk conditions as in nanoscale materials to bulk conditions insensitive to boundaries How do the criteria of classification have to be changed as one goes from one size domain to another Potential for high technological applications also seem to be endless Clusters of otherwise non magnetic materials exhibit magnetic behavior when constrained by size shape and dimension NanoscaIe metal particles exhibit non linear opticaI properties and increased mechanical strength SimiIarly materials made from nanoscale ceramic particIes possess plastic behavior **Springer Handbook of Condensed Matter and Materials Data** Werner Martienssen,Hans Warlimont,2006-09-21 Springer Handbook of Condensed Matter and Materials Data provides a concise compilation of data and functional relationships from the fields of solid state physics and materials in this 1200 page volume The data encapsulated in 914 tables and 1025 illustrations have been selected and extracted primarily from the extensive high quality data collection Landolt B rnstein and also from other systematic data sources and recent publications of physical and technical property data Many chapters are authored by Landolt B rnstein editors including the prominent Springer Handbook editors W Martienssen and H Warlimont themselves The Handbook is designed to be useful as a desktop reference for fast and easy retrieval of essential and reliable data in the lab or office References to more extensive data sources are also provided in the book and by interlinking to the relevant sources on the enclosed CD ROM Physicists chemists and engineers engaged in fields of solid state sciences and materials technologies in research development and application will appreciate the ready access to the key information coherently organized within this wide ranging Handbook From the reviews this is the most complete compilation I have ever seen When I received the book I immediately searched for data I never found elsewhere and I found them rapidly No doubt that this book will soon be in every library and on the desk of most solid state scientists and engineers It will never be at rest Physicalia Magazine

Graphene Science Handbook, Six-Volume Set Mahmood Aliofkhazraei,Nasar Ali,William I. Milne,Cengiz S. Ozkan,Stanislaw Mitura,Juana L. Gervasoni,2016-04-26 Graphene is the strongest material ever studied and can be an efficient substitute for silicon This six volume handbook focuses on fabrication methods nanostructure and atomic arrangement electrical and optical properties mechanical and chemical properties size dependent properties and applications and industrialization There is no other major reference work of this scope on the topic of graphene which is one of the most researched materials of the twenty first century The set includes contributions from top researchers in the field and a foreword written by two Nobel laureates in physics Quasicrystals - Proceedings Of The 5th International Conference C Janot,R Mosseri,1995-12-22 These proceedings cover topics related to Quasicrystals including tiling descriptions high dimensional crystallography structure studies metallurgy and phase diagrams and also properties with special emphasis on dynamics electronic and mechanical behaviour For the first time materials made of metals only that behave as insulators are presented For the first time also application focused research and processing of Quasicrystalline materials are addressed Invited speakers J Friedel D Shechtman M Baake D Basov C Berger M de Boissieu T Fujiwara S Khanna Y Meyer S J Poon C Sire H Trebin A P Tsai M Widdom M Wollgarten Z Zhang **Electronic Structure of Materials** Rajendra Prasad,2013-07-23 Most textbooks in the field are either too advanced for students or don t adequately cover current research topics Bridging this gap Electronic Structure of Materials helps advanced undergraduate and graduate students understand electronic structure methods and enables them to use these techniques in their work Developed from the author s lecture *Hexagonal Boron Nitride* Kalim Deshmukh,Mayank Pandey,Chaudhery Mustansar Hussain,2024-05-31 Hexagonal Boron Nitride Synthesis Properties and Applications offers a comprehensive approach to hexagonal boron nitride h BN covering synthesis exfoliation properties characterization functionalization heterostructures nanocomposites and modelling and simulation and guiding the reader towards advanced applications in biomedicine electronics energy storage wastewater treatment and other areas The book begins by introducing hexagonal boron nitride discussing classification structure synthesis methods exfoliation and functionalization techniques This is followed by in depth coverage of properties and characterization as well as heterostructures and other two dimensional materials as well as nanocomposites The fourth section of the book examines specific target applications covering a range of cutting edge areas including micro and nano electronics anti friction and anti corrosive coatings bone tissue engineering wound healing nanomedicine drug delivery catalysis water treatment energy storage and conversion sensing and bio sensing and fire retardant applications Finally computational modelling and simulation and environmental aspects are addressed in detail This is a valuable resource for researchers and advanced students across nanotechnology materials science chemistry environmental science chemical engineering biomedicine electronics and engineering In an industrial setting this book supports scientists engineers and R D professionals with an interest in advanced 2D materials or nanomaterials for advanced applications Presents the synthesis

properties functionalization and characterization methods for hexagonal boron nitride Explores novel applications across biomedicine electronics energy storage and water treatment Addresses key challenges such as biocompatibility toxicity and environmental and health impact *Electronic Structure of Organic Semiconductors* Luís Alcácer,2018-12-07 Written in the perspective of an experimental chemist this book puts together some fundamentals from chemistry solid state physics and quantum chemistry to help with understanding and predicting the electronic and optical properties of organic semiconductors both polymers and small molecules The text is intended to assist graduate students and researchers in the field of organic electronics to use theory to design more efficient materials for organic electronic devices such as organic solar cells light emitting diodes and field effect transistors After addressing some basic topics in solid state physics a comprehensive introduction to molecular orbitals and band theory leads to a description of computational methods based on Hartree Fock and density functional theory DFT for predicting geometry conformations frontier levels and energy band structures Topological defects and transport and optical properties are then addressed and one of the most commonly used transparent conducting polymers PEDOT PSS is described in some detail as a case study **Catalog of National Bureau of Standards Publications, 1966-1976** United States. National Bureau of Standards. Technical Information and Publications Division,1978 *Catalog of National Bureau of Standards Publications, 1966-1976: Key word index* United States. National Bureau of Standards. Technical Information and Publications Division,1978 Catalog of National Bureau of Standards Publications, 1966-1976 United States. National Bureau of Standards,1978 **Orbital Approach to the Electronic Structure of Solids** Enric Canadell,Marie-Liesse Doublet,Christophe Iung,2012-01-12 This book is aiming at filling the gap between the different languages of the physics and chemistry communities to understand the electronic structure of solids How structure and properties of solids are related is illustrated by considering in detail a large number of real examples **High-Pressure Studies of Crystalline Materials** Daniel Errandonea,2018-08-10 High Pressure Studies of Crystalline Materials *Scientific and Technical Aerospace Reports* ,1972 **Bibliography** Pierre Villars,Karin Cenzual,Marinella Penzo,2012-12-21 By browsing about 10 000 000 scientific articles of over 200 major journals mainly in a cover to cover approach some 200 000 publications were selected The extracted data is part of the following fundamental material research fields crystal structures S phase diagrams also called constitution C and the comprehensive field of intrinsic physical properties P This work has been done systematically starting with the literature going back to 1900 The above mentioned research field codes S C P as well as the chemical systems investigated in each publication were included in the present work The aim of the Inorganic Substances Bibliography is to provide researchers with a comprehensive compilation of all up to now published scientific publications on inorganic systems in only three handy volumes Nuclear Science Abstracts ,1975 Alloys and Intermetallic Compounds Cristina Artini,2017-07-12 This book focuses on the role of modeling in the design of alloys and intermetallic compounds It includes an introduction to the most important and most used

modeling techniques such as CALPHAD and ab initio methods as well as a section devoted to the latest developments in applications of alloys The book emphasizes the correlation between modeling and technological developments while discussing topics such as wettability of Ultra High Temperature Ceramics by metals active brazing of diamonds to metals in cutting tools surface issues in medicine novel Fe based superconductors metallic glasses high entropy alloys and thermoelectric materials **Thermoelectric Nanomaterials** Kunihito Koumoto,Takao Mori,2013-07-20 Presently there is an intense race throughout the world to develop good enough thermoelectric materials which can be used in wide scale applications This book focuses comprehensively on very recent up to date breakthroughs in thermoelectrics utilizing nanomaterials and methods based in nanoscience Importantly it provides the readers with methodology and concepts utilizing atomic scale and nanoscale materials design such as superlattice structuring atomic network structuring and properties control electron correlation design low dimensionality nanostructuring etc Furthermore also indicates the applications of thermoelectrics expected for the large emerging energy market This book has a wide appeal and application value for anyone being interested in state of the art thermoelectrics and or actual viable applications in nanotechnology

Functionalized Nanomaterials for Electronic and Optoelectronic Devices Gopal Rawat,Gautam Patel,Kalim Deshmukh,Chaudhery Mustansar Hussain,2025-09-03 The book gives invaluable insights and expertise from leading researchers on the latest advancements challenges and applications of functionalized nanomaterials Functionalized Nanomaterials for Electronic and Optoelectronic Devices Design Fabrications and Applications examines the current state of the art recent progress new challenges and future perspectives of functionalized nanomaterials in high performance electronic and optoelectronic device applications The book focuses on the synthesis strategies functionalization methods characterizations properties and applications of functionalized nanomaterials in various electronic and optoelectronic devices and the essential criteria in each specified field The physicochemical optical electrical magnetic electronic and surface properties of functionalized nanomaterials are also discussed in detail Additionally the book discusses reliability ethical and legal issues environmental and health impact and commercialization aspects of functionalized nanomaterials as well as essential criteria in each specified field This curated selection of topics and expert contributions from across the globe make this book an outstanding reference source for anyone involved in the field of functionalized nanomaterials based electronic and optoelectronic devices The book gives a comprehensive summary of recent advancements and key technical research accomplishments in the area of electronic optoelectronic device applications of functionalized nanomaterials Functionalized Nanomaterials for Electronic and Optoelectronic Devices serves as a one stop reference for important research in this innovative research field Readers will find this volume Explores technological advances recent trends and various applications of functionalized nanomaterials Provides state of the art knowledge on synthesis processing properties and characterization of functionalized nanomaterials Presents fundamental knowledge and an extensive review on functionalized

nanomaterials especially those designed for electronic device applications Summarizes key challenges future perspectives reliability and commercialization aspects of functionalized nanomaterials in various electronic devices Audience This book will be a very valuable reference source for research scholars graduate students primarily in the field of materials science and engineering nanomaterials and nanotechnology and industry engineers working in the field of functionalized nanomaterials for electronic applications Science and Technology of Chemiresistor Gas Sensors Dinesh K. Aswal,Shiv K. Gupta,2007 Gas sensor technology has advanced remarkably during past few decades and has become one of the indispensable technologies for modern society Varieties of gas sensors are commercially available and using innovative ideas efforts are being made to develop gas sensors of next generation having very small size with very low power consumption The ultimate model for this is probably given by sensory organs of our own body which are implanted finely and work well with a very modest amount of energy In order to achieve this goal it is essential that various aspects of gas sensors are seriously considered These include understanding of gas sensing mechanisms development of new materials and methods to synthesise them into selective sensors innovations in nanostructured materials measurement methods microfabrication of sensors exploring intelligent sensing system etc This book examines these issues pertaining to chemiresistive gas sensors

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