

# Computational Materials Science For Thin Film Solar Cells How To Increase Efficiency

Mesfin A. Kebede, Fabian I. Ezema

#### Computational Materials Science For Thin Film Solar Cells How To Increase Efficiency:

Computational Materials Science for Thin-Film Solar Cells Hans-Werner Schock, Johannes Windeln, 2015-12-06 Scientists and engineers in academic and industrial research experience a strong evolving discipline Computational Materials Science This discipline provides materials insights that are not readily achievable by experiments and it offers the opportunity to design materials and composites ab initio This book presents the methods and the practical use of Computational Materials Science using two distinct examples the development of optimized or alternative materials for CIGS Copper Indium Gallium di Selenide photovoltaics and the optimization of CIGS thin film solar cells for maximum efficiency After a general introduction the theoretical background of the book is illustrated The strategies and principles of High Performance Computing HPC for materials science are covered and rounded out by a number of examples for highly parallel computing Next theory and working principles of solar cells are depicted with emphasis on CIGS Finally the theory of the quantum mechanical simulations Density Functional Theory Monte Carlo simulations for canonical and grand canonical ensembles cluster expansions and the software used for these purposes are presented In the practical section of the book the simulation work for the various functional layers of the CIGS cell is described in detail After general electronic structure calculations for the CIGS photo absorber light is shed on the role of the Indium Gallium distribution as well as on the influence of vacancies in chalcopyrite structures Base requirements for the buffer layer are defined and simulation results from a search for alternative Cadmium free buffer compounds are presented Experimental results for synthesized replacement materials complete this part of the work The optimization of the system transparent conductive oxide TCO contact grid for maximum overall cell efficiency is described The charge transport through TCO grid is modelled by a Finite Element Method and cell efficiencies are calculated considering ohmic as well as optical losses. The last section of the book outlines the simulation results implications on the optimization of thin film cell processing Special emphasis is placed on the influence of process temperatures on film homogeneity and cell efficiency as well as on the requirements for substrate selection The calculations are validated by experimental results **Computational Science and Its Applications -- ICCSA 2013** Beniamino Murgante, Sanjay Misra, Maurizio Carlini, Carmelo Torre, Hong-Quang Nguyen, David Taniar, Bernady O. Apduhan, Osvaldo Gervasi, 2013-06-22 The five volume set LNCS 7971 7975 constitutes the refereed proceedings of the 13th International Conference on Computational Science and Its Applications ICCSA 2013 held in Ho Chi Minh City Vietnam in June 2013 Apart from the general track ICCSA 2013 also include 33 special sessions and workshops in various areas of computational sciences ranging from computational science technologies to specific areas of computational sciences such as computer graphics and virtual reality There are 46 papers from the general track and 202 in special sessions and workshops

**Recent Advances in Thin Film Photovoltaics** Udai P. Singh, Nandu B. Chaure, 2022-09-02 This book provides recent development in thin film solar cells TFSC TFSC have proven the promising approach for terrestrial and space photovoltaics

TFSC have the potential to change the device design and produce high efficiency devices on rigid flexible substrates with significantly low manufacturing cost TFSC have several advantages in manufacturing compared to traditional crystalline Si solar cells like less requirement of materials can be prepared with earth s abundant materials less processing steps easy to dispose etc Several universities research institutes industry in India and abroad are involved in the research area of thin film solar cells The book helps the readers to find the details about different thin film technologies and its advancement at one place Each chapter covers properties of materials its suitability for PV applications simple manufacturing processes and recent and past literature survey The issues related to the development of high efficiencyTFSC devices over large area and its commercial and future prospects are discussed Lithium-Ion Batteries and Solar Cells Ming-Fa Lin, Wen-Dung Hsu, Jow-Lay Huang, 2021-01-17 Lithium Ion Batteries and Solar Cells Physical Chemical and Materials Properties presents a thorough investigation of diverse physical chemical and materials properties and special functionalities of lithium ion batteries and solar cells It covers theoretical simulations and high resolution experimental measurements that promote a full understanding of the basic science to develop excellent device performance Employs first principles and the machine learning method to fully explore the rich and unique phenomena of cathode anode and electrolyte solid and liquid states in lithium ion batteries Develops distinct experimental methods and techniques to enhance the performance of lithium ion batteries and solar cells Reviews syntheses fabrication and measurements Discusses open issues challenges and potential commercial applications This book is aimed at materials scientists chemical engineers and electrical engineers developing enhanced batteries and solar cells for peak performance Leveraging AI for Innovative Sustainable Energy: Solar, Wind and Green Hydrogen Hammouch, Hind, Razzak Janjua, Laeeg, 2025-05-15 Artificial intelligence AI and intelligent technologies play a vital role in transforming the energy sector which is key to delivering lower carbon footprints combined with increased levels of security AI driven innovations in solar wind energy green hydrogen generation increase efficiency to achieve further sustainability Furthermore the disruptive impact of AI based solutions in the energy sector is informative for initiating more sustainable industrial and commercial purposes and practices worldwide Thus AI enabled systems and their capabilities in generation distribution of energy and consumption can contribute to helping build more robust and greener infrastructures for our resources Leveraging AI for Innovative Sustainable Energy Solar Wind and Green Hydrogen offers practical steps for incorporating green hydrogen into established energy systems that can help to realize net zero emissions targets It inspires innovation by detailing the experiences of real life case studies and presenting forward looking viewpoints that make collaboration between various sectors possible all towards embracing renewable energy solutions on a global scale Covering topics such as hydrogen power marketing strategies and public education campaigns this book is an excellent resource for environmental advocates sustainability practitioners policymakers manufacturers industry leaders professionals researchers scholars academicians and more U.S. Climate Change Technology Program Climate Change Technology

Program (U.S.), 2006 Advances in Composite Materials for Medicine and Nanotechnology Brahim Attaf, 2011-04-01 Due to their good mechanical characteristics in terms of stiffness and strength coupled with mass saving advantage and other attractive physico chemical properties composite materials are successfully used in medicine and nanotechnology fields To this end the chapters composing the book have been divided into the following sections medicine dental and pharmaceutical applications nanocomposites for energy efficiency characterization and fabrication all of which provide an invaluable overview of this fascinating subject area The book presents in addition some studies carried out in orthopedic and stomatological applications and others aiming to design and produce new devices using the latest advances in nanotechnology This wide variety of theoretical numerical and experimental results can help specialists involved in these disciplines to enhance competitiveness and innovation **Electrode Materials for Energy Storage and Conversion** Mesfin A. Kebede, Fabian I. Ezema, 2021-11-16 This book provides a comprehensive overview of the latest developments and materials used in electrochemical energy storage and conversion devices including lithium ion batteries sodium ion batteries zinc ion batteries supercapacitors and conversion materials for solar and fuel cells Chapters introduce the technologies behind each material in addition to the fundamental principles of the devices and their wider impact and contribution to the field This book will be an ideal reference for researchers and individuals working in industries based on energy storage and conversion technologies across physics chemistry and engineering FEATURES Edited by established authorities with chapter contributions from subject area specialists Provides a comprehensive review of the field Up to date with the latest developments and research Editors Dr Mesfin A Kebede obtained his PhD in Metallurgical Engineering from Inha University South Korea He is now a principal research scientist at Energy Centre of Council for Scientific and Industrial Research CSIR South Africa He was previously an assistant professor in the Department of Applied Physics and Materials Science at Hawassa University Ethiopia His extensive research experience covers the use of electrode materials for energy storage and energy conversion Prof Fabian I Ezema is a professor at the University of Nigeria Nsukka He obtained his PhD in Physics and Astronomy from University of Nigeria Nsukka His research focuses on several areas of materials science with an emphasis on energy applications specifically electrode materials for energy conversion and storage NASA Technical Memorandum Advanced Concepts in Photovoltaics Arthur J. Nozik, Gavin Conibeer, Matthew C Beard, 2014-07-10 Photovoltaic ,1990 systems enable the sun s energy to be converted directly into electricity using semiconductor solar cells The ultimate goal of photovoltaic research and development is to reduce the cost of solar power to reach or even become lower than the cost of electricity generated from fossil and nuclear fuels. The power conversion efficiency and the cost per unit area of the phototvoltaic system are critical factors that determine the cost of photovoltaic electricity Until recently the power conversion efficiency of single junction photovoltaic cells has been limited to approximately 33% the socalled Shockley Queisser limit This book presents the latest developments in photovoltaics which seek to either reach or surpass the Shockley Queisser limit and to lower the cell cost per unit area Progress toward this ultimate goal is presented for the three generations of photovoltaic cells the 1st generation based on crystalline silicon semiconductors the 2nd generation based on thin film silicon compound semiconductors amorphous silicon and various mesoscopic structures and the 3rd generation based on the unique properties of nanoscale materials new inorganic and organic photoconversion materials highly efficient multi junction cells with low cost solar concentration and novel photovoltaic processes The extent to which photovoltaic materials and processes can meet the expectations of efficient and cost effective solar energy conversion to electricity is discussed Written by an international team of expert contributors and with researchers in academia national research laboratories and industry in mind this book is a comprehensive guide to recent progress in photovoltaics and essential for any library or laboratory in the field

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