IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re Patent of:	Yasuharu Hosaka et al.		
U.S. Patent No.:	9,298,057	Attorney Docket No.:	12732-1925IP1
Issue Date:	March 29, 2016		
Appl. Serial No.:	13/939,323		
Filing Date:	July 11, 2013		
Title:	DISPLAY DEVICE AND ELECTRONIC DEVICE INCLUDING THE DISPLAY DEVICE		

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Patent Trial and Appeal Board
U.S. Patent and Trademark Office
P.O. Box 1450
Alexandria, VA 22313-1450

Declaration of Jacob Robert Munford

1. My name is Jacob Robert Munford. I am over the age of 18, have personal knowledge of the facts set forth herein, and am competent to testify to the same.

2. I earned a Master of Library and Information Science (MLIS) from the University of Wisconsin-Milwaukee in 2009. I have over ten years of experience in the library/information science field. Beginning in 2004, I have served in various positions in the public library sector including Assistant Librarian, Youth Services Librarian and Library Director. I have attached my Curriculum Vitae as Appendix A.

3. During my career in the library profession, I have been responsible for materials acquisition for multiple libraries. In that position, I have cataloged, purchased and processed incoming library works. That includes purchasing materials directly from vendors, recording publishing data from the material in question, creating detailed material records for library catalogs and physically preparing that material for circulation. In addition to my experience in acquisitions, I was also responsible for analyzing large collections of library materials, tailoring library records for optimal catalog

search performance and creating lending agreements between libraries during my time as a Library Director.

4. I am fully familiar with the catalog record creation process in the library sector. In preparing a material for public availability, a library catalog record describing that material would be created. These records are typically written in Machine Readable Catalog (herein referred to as MARC) code and contain information such as a physical description of the material, metadata from the material's publisher and date of library acquisition. In particular, the 008 field of the MARC record is reserved for denoting the creation of the library record itself. As this typically occurs during the process of preparing materials for public access, it is my experience that an item's MARC record accurately indicates the date of an item's public availability.

5. I have reviewed Exhibit SEL2004, a book by John F. Wager entitled *Transparent Electronics* published by Springer in 2008.

6. Attached hereto as Appendix WA01 is a true and correct copy of scans of the cover, publishing data, title page and table of contents for *Transparent*

Electronics from the University of Pittsburgh. I secured these scans from the library's onsite holdings.

7. In comparing Appendix WA01 to Exhibit SEL2004, it is my determination that Exhibit SEL2004 is a true and correct copy of *Transparent Electronics* by John F. Wager.

8. Attached hereto as Appendix WA02 is a true and correct copy of the MARC record for *Transparent Electronics* from the University of Pittsburgh's library. I secured this record from the library's online catalog.

9. The 008 field of *Transparent Electronics* MARC record included in Appendix WA02 indicates that *Transparent Electronics* was first recorded by University of Pittsburgh as of June 19, 2008. Based on this information, it is my determination that *Transparent Electronics* would have been made accessible and publicly available soon after it was received on June 19, 2008.

10. I have reviewed Exhibit SEL2008, a book by S.M. Sze entitled *Physics of Semiconductor Devices* published by Wiley in 1981.

11. Attached hereto as Appendix SZ01 is a true and correct copy of scans of the cover, publishing data, title page and table of contents for *Physics of Semiconductor Devices* from the University of Pittsburgh. I secured these scans from the library's onsite holdings.

12. In comparing Appendix SZ01 to Exhibit SEL2008, it is my determination that Exhibit SEL2008 is a true and correct copy of *Physics of Semiconductor Devices* by S.M. Sze.

13. Attached hereto as Appendix SZ02 is a true and correct copy of the MARC record for *Physics of Semiconductor Devices* from the University of Pittsburgh's library. I secured this record from the library's online catalog.

14. The 008 field of *Physics of Semiconductor Devices* MARC record included in Appendix SZ02 indicates that *Physics of Semiconductor Devices* was first recorded by University of Pittsburgh as of January 26, 1981. Based on this information, it is my determination that *Physics of Semiconductor Devices* would have been made accessible and publicly available soon after it was received on January 26, 1981.

15. I have reviewed Exhibit SEL2009, a book by Jean-Pierre Colinge entitled *Physics of Semiconductor Devices* published by Springer in 2006.

16. Attached hereto as Appendix CO01 is a true and correct copy of scans of the cover, publishing data, title page and table of contents for *Physics of Semiconductor Devices* from Carnegie-Mellon University. I secured these scans from the library's onsite holdings.

17. In comparing Appendix CO01 to Exhibit SEL2009, it is my determination that Exhibit SEL2009 is a true and correct copy of *Physics of Semiconductor Devices* by Jean-Pierre Colinge.

18. Attached hereto as Appendix CO02 is a true and correct copy of the MARC record for *Physics of Semiconductor Devices* from Carnegie-Mellon University's library. I secured this record from the library's online catalog.

19. The 008 field of *Physics of Semiconductor Devices* MARC record included in Appendix CO02 indicates that *Physics of Semiconductor Devices* was first recorded by Carnegie-Mellon University as of January 19, 2006. Based on this information, it is my determination that *Physics of Semiconductor*

Devices would have been made accessible and publicly available soon after it was received on January 19, 2006.

20. I have reviewed Exhibit SEL2010, a book edited by John Daintith entitled *A Dictionary of Chemistry* published by Oxford University Press in 2008.

21. Attached hereto as Appendix DA01 is a true and correct copy of scans of the cover, publishing data, title page and table of contents for *A Dictionary of Chemistry* from the Carnegie Library of Pittsburgh. I secured these scans from the library's onsite holdings.

22. In comparing Appendix DA01 to Exhibit SEL2010, it is my determination that Exhibit SEL2010 is a true and correct copy of *A Dictionary of Chemistry* by John Daintith.

23. Attached hereto as Appendix DA02 is a true and correct copy of the MARC record for *A Dictionary of Chemistry* from the Carnegie Library of Pittsburgh's library. I secured this record from the library's online catalog.

24. The 008 field of *A Dictionary of Chemistry* MARC record included in Appendix DA02 indicates that *A Dictionary of Chemistry* was first recorded

by the Carnegie Library of Pittsburgh as of June 26, 2008. Based on this information, it is my determination that *A Dictionary of Chemistry* would have been made accessible and publicly available soon after it was received on June 26, 2008.

25. I have reviewed Exhibit SEL2011, a book entitled *McGraw-Hill Dictionary of Scientific and Technical Terms* published by McGraw-Hill in 2002.

26. Attached hereto as Appendix MC01 is a true and correct copy of the MARC record for *McGraw-Hill Dictionary of Scientific and Technical Terms* from George Mason University's library. I secured this record from the library's online catalog.

27. In comparing the description included within the MARC record of Appendix MC01 to Exhibit SEL2011, it is my determination that Exhibit SEL2011 is a true and correct copy of *McGraw-Hill Dictionary of Scientific and Technical Terms*.

28. The 008 field of *McGraw-Hill Dictionary of Scientific and Technical Terms* MARC record included in Appendix MC01 indicates that *McGraw-Hill*

Dictionary of Scientific and Technical Terms was first recorded by George Mason University as of June 19, 2002. Based on this information, it is my determination that *McGraw-Hill Dictionary of Scientific and Technical Terms* would have been made accessible and publicly available soon after it was received on June 19, 2002.

29. I have been retained on behalf of the Patent Owner to provide assistance in the above-illustrated matter in establishing the authenticity and public availability of the documents discussed in this declaration. I am being compensated for my services in this matter at the rate of $100.00 per hour plus reasonable expenses. My statements are objective, and my compensation does not depend on the outcome of this matter.

30. I declare under penalty of perjury that the foregoing is true and correct. I hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements were made the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under Section 1001 of Title 18 of the United States Code.

Dated: 12/5/18

Jacob Robert Munford

APPENDIX A

IPR2018-01405

Appendix A - Curriculum Vitae

Education

University of Wisconsin-Milwaukee - MS, Library & Information Science, 2009
Milwaukee, WI

- Coursework included cataloging, metadata, data analysis, library systems, management strategies and collection development.
- Specialized in library advocacy and management.

Grand Valley State University - BA, English Language & Literature, 2008
Allendale, MI

- Coursework included linguistics, documentation and literary analysis.
- Minor in political science with a focus in local-level economics and government.

Professional Experience

Library Director, February 2013 - March 2015
Dowagiac District Library
Dowagiac, Michigan

- Executive administrator of the Dowagiac District Library. Located in Southwest Michigan, this library has a service area of 13,000, an annual operating budget of over $400,000 and total assets of approximately $1,300,000.
- Developed careful budgeting guidelines to produce a 15% surplus during the 2013-2014 & 2014-2015 fiscal years.
- Using this budget surplus, oversaw significant library investments including the purchase of property for a future building site, demolition of existing buildings and building renovation projects on the current facility.
- Led the organization and digitization of the library's archival records.
- Served as the public representative for the library, developing business relationships with local school, museum and tribal government entities.

- Developed an objective-based analysis system for measuring library services - including a full collection analysis of the library's 50,000+ circulating items and their records.

November 2010 - January 2013
Librarian & Branch Manager, Anchorage Public Library
Anchorage, Alaska

- Headed the 2013 Anchorage Reads community reading campaign including event planning, staging public performances and creating marketing materials for mass distribution.
- Co-led the social media department of the library's marketing team, drafting social media guidelines, creating original content and instituting long-term planning via content calendars.
- Developed business relationships with The Boys & Girls Club, Anchorage School District and the US Army to establish summer reading programs for children.

June 2004 - September 2005, September 2006 - October 2013
Library Assistant, Hart Area Public Library
Hart, MI

- Responsible for verifying imported MARC records and original MARC cataloging for the local-level collection as well as the Michigan Electronic Library.
- Handled OCLC Worldcat interlibrary loan requests & fulfillment via ongoing communication with lending libraries.

Professional Involvement

Alaska Library Association - Anchorage Chapter

- Treasurer, 2012

Library Of Michigan

- Level VII Certification, 2008
- Level II Certification, 2013

Michigan Library Association Annual Conference 2014

- New Directors Conference Panel Member

Southwest Michigan Library Cooperative

- Represented the Dowagiac District Library, 2013-2015

Professional Development

Library Of Michigan Beginning Workshop, May 2008
Petoskey, MI

- Received training in cataloging, local history, collection management, children's literacy and reference service.

Public Library Association Intensive Library Management Training, October 2011
Nashville, TN

- Attended a five-day workshop focused on strategic planning, staff management, statistical analysis, collections and cataloging theory.

Alaska Library Association Annual Conference 2012 - Fairbanks, February 2012
Fairbanks, AK

- Attended seminars on EBSCO advanced search methods, budgeting, cataloging, database usage and marketing.

APPENDIX WA01

IPR2018-01405

Douglas A. Keszler
Rick E. Presley

Transparent Electronics

Springer


Wager · Keszler · Presley
Transparent Electronics

John F. Wager
Douglas A. Keszler
Rick E. Presley

Transparent Electronics

Transparent electronics is an emerging technology that employs wide band-gap semiconductors for the realization of invisible circuits. This monograph provides the first roadmap for transparent electronics, identifying where the field is, where it is going, and what needs to happen to move it forward. Although the central focus of this monograph involves transparent electronics, many of the materials, devices, circuits, and process integration strategies discussed herein will be of great interest to researchers working in other emerging fields of optoelectronics and electronics involving printing, large areas, low cost, flexibility, wearability, and fashion and design.

ISBN 978-0-387-72341-9

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Transparent Electronics

Transparent Electronics

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Table of Contents

ent electronics 'killer apps' are admittedly either not yet well-defined or are presently unrealizable due to current limitations in transparent electronics or in a requisite auxiliary technology. However, this topical ordering inversion is meant to be intentionally provocative. Since transparent electronics is a nascent technology, we believe that its development will be most rapidly and efficiently accomplished if it is strongly application-driven, and if it is undertaken in a parallel fashion in which materials, devices, circuits, and system development are pursued concurrently. Hopefully, such a product-driven concurrent development strategy will lead to rapid technology assessment, the identification of new and most-likely unexpected applications, and an expeditious commercial deployment of this technology.

1.2 Pre-history

Two primary technologies which preceded and underlie transparent electronics are briefly overviewed. These topics are transparent conductive oxides (TCOs) and thin-film transistors (TFTs).

1.2.1 Transparent conducting oxides (TCOs)

TCOs constitute an unusual class of materials possessing two physical properties - high optical transparency and high electrical conductivity - that are generally considered to be mutually exclusive (Hartnagel et al. 1995). This peculiar combination of physical properties is only achievable if a material has a sufficiently large energy band gap so that it is non-absorbing or transparent to visible light, i.e., > ~3.1 eV, and also possesses a high enough concentration of electrical carriers, i.e., an electron or hole concentration > $\sim 10^{19}$ cm^{-3}, with a sufficiently large mobility, > ~1 cm^2 $V^{-1}s^{-1}$, that the material can be considered to be a 'good' conductor of electricity.

The three most common TCOs are indium oxide In_2O_3, tin oxide SnO_2, and zinc oxide ZnO, the basic electrical properties of which are summarized in Table 1.1. All three of these materials have band gaps above that required for transparency across the full visible spectrum.

Note that although the TCOs listed in Table 1.1 are considered to be 'good' conductors from the perspective of a semiconductor, they are actually very poor conductors compared to metals. For example, the conductivities of tungsten W, aluminum Al, and copper Cu, are approximately 100,000, 350,000, and 600,000 S cm^{-1}, indicating that the best In_2O_3 conductivity (for indium tin oxide or ITO) is about a factor of 10 to 60 lower than that of a typical integrated circuit contact metal. The low conductance of TCOs compared to metals has important consequences for both TCO and transparent electronics applications, some of which are explored in this book. The theoretical absolute limit of the conductivity for a TCO has been estimated to be 25,000 S cm^{-1} (Bellingham 1992).

Table 1.1. Electrical properties of common transparent conducting oxides (TCOs) Conductivities reported are for best-case polycrystalline films.

Material	Bandgap (eV)	Conductivity (S cm^{-1})	Electron concentration (cm^{-3})	Mobility (cm^2 V^{-1} s^{-1})
In_2O_3	3.75	10,000	$>10^{21}$	35
ZnO	3.35	8,000	$>10^{21}$	20
SnO_2	3.6	5,000	$>10^{20}$	15

Returning to Table 1.1, notice that all three of the TCOs included in this table are n-type, i.e., conductivity is a consequence of electron transport, and that the electron carrier concentration is strongly degenerate, i.e., the electron density exceeds that of the conduction effective band density of states by an appreciable amount (Pierret 1996; Sze and Ng 2007). All of the well-known and commercially relevant TCOs are n-type. p-type TCOs are a relatively new phenomenon and their conductivity performance is quite poor compared to that of n-type TCOs. To a large extent, the poor conductivity of p-type TCOs is due to the very low mobility of these materials, typically less than ~1 cm^2 V^{-1}s^{-1}, compared to mobilities in the range of ~10-40 cm^2 V^{-1}s^{-1} for n-type TCOs.

The n-type mobilities indicated in Table 1.1 are quite small compared to those representative single crystal silicon materials and devices, which range from ~250-1,500 cm^2 V^{-1}s^{-1}. However, this mobility comparison between TCOs and single crystal silicon is a bit misleading since single crystal silicon mobility is not usually specified at doping concentrations as large as those typical of TCOs. In fact, it is reported that single crystal silicon mobility is independent of doping concentration above ~10^{19} cm^{-3}, with an electron mobility of ~90 cm^2 V^{-1}s^{-1} and a hole mobility of ~50 cm^2 V^{-1}s^{-1} (Baliga 1995). A low mobility at high carrier concentrations is, to a large extent, a consequence of intense ionized impurity scattering associated with high doping concentrations (Hartnagel et al.1995).

DATE DUE

APPENDIX WA02

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Transparent electronics John F. Wager, Douglas A. Keszler, Rick E. Presley.

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042 __ **|a** lccopycat

050 00 **|a** TK7835 **|b** .W284 2008

082 04 **|a** 621.38152 **|2** 22

100 1_ **|a** Wager, John F. **|q** (John Fisher)

245 10 **|a** Transparent electronics **|h** [electronic resource] / **|c** John F. Wager, Douglas A. Keszler, Rick E. Presley.

260 __ **|a** New York : **|b** Springer, **|c** c2008.

300 __ **|a** viii, 212 p. ; **|b** ill. ; **|c** 24 cm.

504 __ **|a** Includes bibliographical references (p. [189]-208) and index.

505 00 **|g** 1.1 **|t** A technology in a hurry **|g** 1 -- **|g** 1.2 **|t** Pre-history **|g** 2 -- **|g** 1.2.1 **|t** Transparent conducting oxides (TCOs) **|g** 2 -- **|g** 1.2.2 **|t** Thin-film transistors (TFTs) **|g** 5 -- **|g** 1.3 **|t** The stage is now set **|g** 8 -- **|g** 2 **|t** A Review of Prior Work **|g** 9 -- **|g** 2.1 **|t** Origins **|g** 9 -- **|g** 2.1.1 **|t** Transparent electronics -- 2003 **|g** 13 -- **|g** 2.1.2 **|t** Transparent electronics -- 2004 **|g** 17 -- **|g** 2.1.3 **|t** Transparent electronics -- 2005 **|g** 25 -- **|g** 2.1.4 **|t** Transparent electronics -- 2006 **|g** 30 -- **|g** 2.2 **|t** Perspective & Outlook **|g** 37 -- **|g** 3 **|t** Applications **|g** 39 -- **|g** 3.1 **|t** Looking into a crystal ball **|g** 39 -- **|g** 3.2 **|t** A technology appraisal **|g** 39 -- **|g** 3.3 **|t** An application smorgasbord **|g** 44 -- **|g** 3.4 **|t** Applications in retrospective **|g** 56 -- **|g** 4 **|t** Materials **|g** 57 -- **|g** 4.1 **|t** Device components **|g** 57 -- **|g** 4.2 **|t** n-type semiconductor channel materials **|g** 58 -- **|g** 4.3 **|t** Amorphous oxide semiconductors **|g** 67 -- **|g** 4.4 **|t** p-type semiconductors **|g** 71 -- **|g** 4.4.1 **|t** Copper oxides and chalcogenides **|g**

520 __ **|a** "Transparent electronics is an emerging technology that employs wide band-gap semiconductors for the realization of invisible circuits. This monograph provides the first roadmap for transparent electronics, identifying where the field is, where it is going, and what needs to happen to move it forward. Although the central focus of this monograph involves transparent electronics, many of the materials, devices, circuits, and process-integration strategies discussed herein will be of great interest to researchers working in other emerging fields of optoelectronics and electronics involving printing, large areas, low cost, flexibility, wearability, and fashion and design." - Back cover.

650 _0 **|a** Transparent electronics.

700 1_ **|a** Keszler, Douglas A., **|d** 1957-

700 1_ **|a** Presley, Rick E.

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APPENDIX SZ01

IPR2018-01405


PHYSICS OF
SEMICONDUCTOR
DEVICES
SZE
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S988
1981

Physics of Semiconductor Devices

SECOND EDITION

S. M. Sze
Bell Laboratories, Incorporated
Murray Hill, New Jersey

A WILEY-INTERSCIENCE PUBLICATION
JOHN WILEY & SONS
New York • Chichester • Brisbane • Toronto • Singapore

Library of Congress Cataloging in Publication Data:

Sze, S. M., 1936-
Physics of semiconductor devices.

"A Wiley-Interscience publication."
Includes index.
1. Semiconductors. I. Title.

TK7871.85.S988 1981 537.6'22 81-213
ISBN 0-471-05661-8 AACR2

Printed in the United States of America

10

To My Wife


3-12-83 QEX 84/732

Contents

be efficiently converted in the low-gap semiconductor. Figure 23 shows the normalized spectral responses of several $Ga_{1-x}Al_xAs$–GaAs solar cells, all having the same junction depths and doping levels. As the composition x increases, the bandgap E_{g1} increases; therefore, the spectral response extends to higher photon energies.

One interesting heterojunction solar cell is the conducting glass–semiconductor heterojunction. The conducting glasses include oxide semiconductors, such as indium oxide (In_2O_3, with $E_g = 3.5$ eV and electron affinity $\chi = 4.45$ eV), tin oxide (SnO_2, with $E_g = 3.5$ eV and electron affinity $\chi = 4.8$ eV), and the indium tin oxide (ITO, a mixture of In_2O_3 and SnO_2, with $E_g = 3.7$ eV and electron affinity $\chi = 4.2$ to 4.5 eV). These oxide semiconductors in thin-film form have the unique properties of good electrical conductivity and high optical transparency. They serve not only as part of the heterojunction but also as an antireflection coating.

The energy-band diagrams for an ITO/Si solar cell are shown[29] in the insert of Fig. 24. The top layer is an n-type 4000 Å ITO with 5×10^{-4} Ω–cm and the substrate is a 2 Ω–cm p-type silicon. The curves in Fig. 24 near 1 mA/cm^2 are all parallel to each other. The slope $d(\ln J)/dV$ is about 24 V^{-1} independent of temperature. This slope suggests a multistep tunnel process in this heterojunction. Conversion efficiencies in the 12 to 15% range

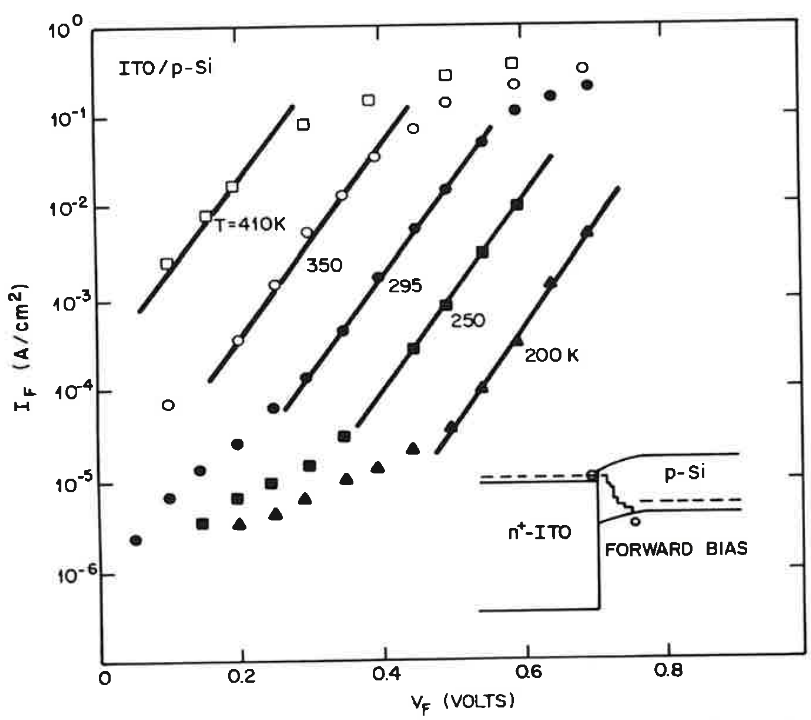

Fig. 24 Current–voltage characteristics of a ITO-Si heterojunction. The insert shows the band diagram under forward bias. (After Sites, Ref. 29.)

APPENDIX SZ02

IPR2018-01405

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Physics of semiconductor devices / S.M. Sze.

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090 __ **|a** TK7871.85 **|b** .S988 1981 **|m** PIJD
100 1_ **|a** Sze, S. M., **|d** 1936-
245 10 **|a** Physics of semiconductor devices / **|c** S.M. Sze.
250 __ **|a** 2nd ed.
260 __ **|a** New York : **|b** Wiley, **|c** c1981.
300 __ **|a** xii, 868 p. : **|b** ill. ; **|c** 24 cm.
500 __ **|a** "A Wiley-Interscience publication."
504 __ **|a** Includes bibliographical references and index.
650 _0 **|a** Semiconductors.

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APPENDIX CO01

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PHYSICS OF SEMICONDUCTOR DEVICES

Jean-Pierre Colinge
Cynthia A. Colinge

Springer

PHYSICS OF SEMICONDUCTOR DEVICES

Colinge / Colinge

PHYSICS OF SEMICONDUCTOR DEVICES is a textbook aimed at college undergraduate and graduate teaching. It covers both basic classic topics such as energy band theory and the gradual-channel model of the MOSFET as well as advanced concepts and devices such as MOSFET short-channel effects, low-dimensional devices and single-electron transistors. As a prerequisite, this text requires mathematics through differential equations and modern physics where students are introduced to quantum mechanics. Concepts are introduced to the reader in a simple way, often using comparisons to everyday-life experiences such as simple fluid mechanics. They are explained in depth and mathematical developments are fully described.

PHYSICS OF SEMICONDUCTOR DEVICES contains a list of problems that can be used as homework assignments or can be solved in class to exemplify the theory. Many of these problems make use of Matlab and are aimed at illustrating theoretical concepts in a graphical manner. A series of these Matlab problems is based on a simple finite-element solution of semiconductor equations. These yield the exact solution to equations that have no analytical solutions and are usually solved using approximations, such as the depletion approximation. The exact numerical solution can then be graphically compared to the solution using the approximation.

The different chapters of *PHYSICS OF SEMICONDUCTOR DEVICES* cover the following material:

1 - Energy Band Theory
2 - Theory of Electrical Conduction
3 - Generation/Recombination Phenomena
4 - The PN Junction Diode
5 - Metal-semiconductor contacts
6 - JFET and MESFET
7 - The MOS Transistor
8 - The Bipolar Transistor
9 - Heterojunction Devices
10 - Quantum-Effect Devices
11 - Semiconductor Processing

C.A. Colinge is Professor of Electrical and Electronic Engineering at the California State University, Sacramento.

J.P. Colinge is Professor in the Department of Electrical and Computer Engineering of the University of California, Davis.

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PHYSICS OF SEMICONDUCTOR DEVICES

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Department of Electrical [illegible] Engineering
[illegible]

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PHYSICS OF SEMICONDUCTOR DEVICES

by

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Department of Electrical and Computer Engineering
University of California, Davis

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California State University

Springer

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CONTENTS

$$= \frac{N}{2\pi/(a+b)} = \frac{N(a+b)}{2\pi} = \frac{L}{2\pi} \qquad (1.1.32)$$

In the case of a three-dimensional crystal, energy band calculations are, of course, much more complicated, but the essential results obtained from the one-dimensional calculation still hold. In particular, there exist permitted energy bands separated by forbidden energy gaps. The 3-D volume of the first Brillouin zone is $8\pi^3N/V$, where V is the volume of the crystal, the number of wave vectors is equal to the number of elementary crystal lattice cells, N. The density of wave vectors is given by:

$$n(k) = density\ of\ \mathbf{k} = \frac{number\ of\ \mathbf{k}\text{-}vectors}{volume\ of\ the\ zone} = \frac{NV}{8\pi^3 N} = \frac{V}{8\pi^3} \qquad (1.1.33)$$

1.1.4. Valence band and conduction band

Chemical reactions originate from the exchange of electrons from the outer electronic shell of atoms. Electrons from the most inner shells do not participate in chemical reactions because of the high electrostatic attraction to the nucleus. Likewise, the bonds between atoms in a crystal, as well as electric transport phenomena, are due to electrons from the outermost shell. In terms of energy bands, the electrons responsible for forming bonds between atoms are found in the last occupied band, where electrons have the highest energy levels for the ground-state atoms. However, there is an infinite number of energy bands. The first (lowest) bands contain core electrons such as the 1s electrons which are tightly bound to the atoms. The highest bands contain no electrons. The last ground-state band which contains electrons is called the *valence band*, because it contains the electrons that form the -often covalent- bonds between atoms.

The permitted energy band directly above the valence band is called the *conduction band*. In a semiconductor this band is empty of electrons at low temperature ($T=0K$). At higher temperatures, some electrons have enough thermal energy to quit their function of forming a bond between atoms and circulate in the crystal. These electrons "jump" from the valence band into the conduction band, where they are free to move. The energy difference between the bottom of the conduction band and the top of the valence band is called "forbidden gap" or "bandgap" and is noted E_g.

In a more general sense, the following situations can occur depending on the location of the atom in the periodic table (Figure 1.11):

A: The last (valence) energy band is only partially filled with electrons, even at $T=0K$.

B: The last (valence) energy band is completely filled with electrons at $T=0K$, but the next (empty) energy band overlaps with it (*i.e.*: an empty energy band shares a range of common energy values; $E_g < 0$).

C: The last (valence) energy band is completely filled with electrons and no empty band overlaps with it ($E_g > 0$).

In cases A and B, electrons with the highest energies can easily acquire an infinitesimal amount of energy and jump to a slightly higher permitted energy level, and move through the crystal. In other words, electrons can leave the atom and move in the crystal without receiving any energy. A material with such a property is a ***metal***. In case C, a significant amount of energy (equal to E_g or higher) has to be transferred to an electron in order for it to "jump" from the valence band into a permitted energy level of the conduction band. This means that an electron must receive a significant amount of energy before leaving an atom and moving "freely" in the crystal. A material with such properties is either an ***insulator*** or a ***semiconductor***.

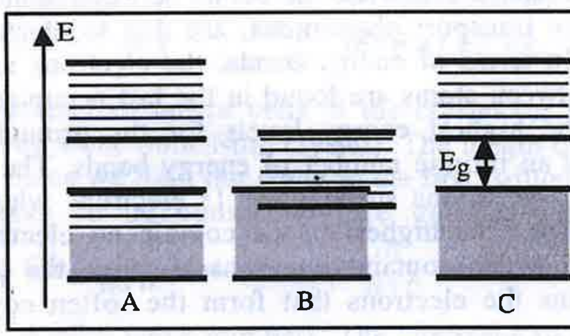

Figure 1.11: Valence band (bottom) and conduction band in a metal (A and B) and in a semiconductor or an insulator (C).[6]

The distinction between an insulator and a semiconductor is purely quantitative and is based on the value of the energy gap. In a semiconductor E_g is typically smaller than 2 eV and room-temperature thermal energy or excitation from visible-light photons can give electrons enough energy for "jumping" from the valence into the conduction band. The energy gap of the most common semiconductors are: 1.12 eV (silicon), 0.67 eV (germanium), and 1.42 eV (gallium arsenide). Insulators have significantly wider energy bandgaps: 9.0 eV (SiO_2), 5.47 eV (diamond), and 5.0 eV (Si_3N_4). In these materials room-temperature thermal energy is not large enough to place electrons in the conduction band.

APPENDIX CO02

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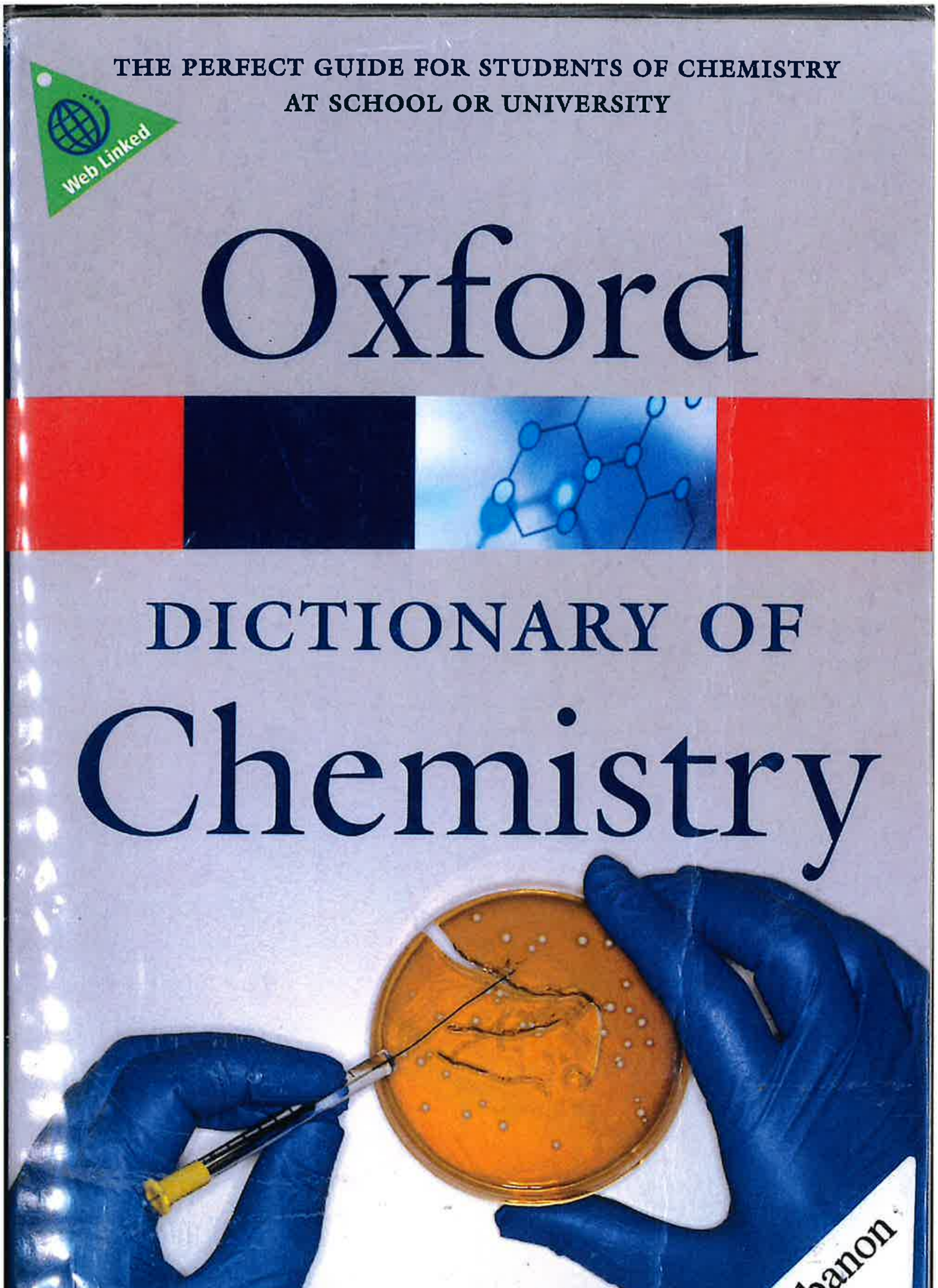
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5

Contents

effect. *See also* INVERSE COMPTON EFFECT.

computational chemistry The use of computers in chemical research. With the increase in processing power of computers, calculations on individual molecules and on chemical systems have become important tools for research and industrial development. With simple molecules, predictions can be made about electronic structure and properties using *ab-initio calculations. For more complex molecules *semi-empirical calculations are used. The field has been particularly expanded by the *density-functional method of treating large molecules and by the availability of software for analysing molecular behaviour and structure. *See also* MOLECULAR MODELLING.

concentrated Describing a solution that has a relatively high concentration of solute.

concentration The quantity of dissolved substance per unit quantity of a solution. Concentration is measured in various ways. The amount of substance dissolved per unit volume of the solution (symbol *c*) has units of mol dm^{-3} or mol l^{-1}. It is now called amount concentration (formerly **molarity**). The **mass concentration** (symbol ρ) is the mass of solute per unit volume of solution. It has units of kg dm^{-3}, g cm^{-3}, etc. The **molality** is the amount of substance per unit mass of solvent, commonly given in units of mol kg^{-1}. *See also* MOLE FRACTION.

concentration cell *See* CELL.

concentration gradient (diffusion gradient) The difference in concentration between a region of a solution or gas that has a high density of particles and a region that has a relatively lower density of particles. By random motion, particles will move from the area of high concentration towards the area of low concentration, by the process of *diffusion, until the particles are evenly distributed in the solution or gas.

concerted reaction A type of reaction in which there is only one stage rather than a series of steps. The S_N2 mechanism in *nucleophilic substitutions is an example. *See also* PERICYCLIC REACTIONS.

condensation The change of a vapour or gas into a liquid. The change of phase is accompanied by the evolution of heat (*see* LATENT HEAT).

condensation polymerization *See* POLYMER.

condensation pump *See* DIFFUSION PUMP.

condensation reaction A chemical reaction in which two molecules combine to form a larger molecule with elimination of a small molecule (e.g. H_2O). *See* ALDEHYDES; KETONES.

condenser A device used to cool a vapour to cause it to condense to a liquid. *See* LIEBIG CONDENSER.

conducting polymer An organic polymer that conducts electricity. Conducting polymers have a crystalline structure in which chains of conjugated unsaturated carbon–carbon bonds are aligned. Examples are polyacetylene and polypyrrole. There has been considerable interest in the development of such materials because they would be cheaper and lighter than metallic conductors. They do, however, tend to be chemically unstable and, so far, no commercial conducting polymers have been developed.

conductiometric titration A type of titration in which the electrical conductivity of the reaction mixture is continuously monitored as one reactant is added. The equivalence point is the point at which this undergoes a sudden change. The method is used for titrating coloured solutions, which cannot be used with normal indicators.

conduction band *See* ENERGY BANDS.

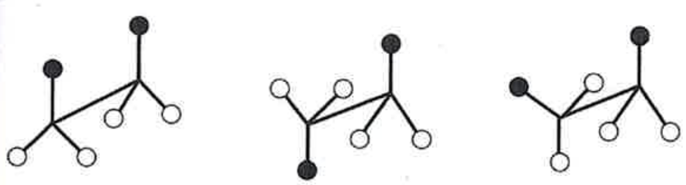
conductivity water *See* DISTILLED WATER.

Condy's fluid A mixture of calcium and potassium permanganates (manganate(VII)) used as an antiseptic.

configuration **1.** The arrangement of atoms or groups in a molecule. **2.** The arrangement of electrons about the nucleus of an *atom.

configuration space The *n*-dimensional space with coordinates $(q_1,q_2,\ldots,q_n)$ associated with a system that has *n* degrees of freedom, where the values *q* describe the degrees of freedom. For example, in a gas of *N* atoms each atom has three positional coordinates, so the configuration space is 3*N*-dimensional. If the particles also have internal degrees of freedom, such as those caused by vibration and rotation in a molecule, then these must be included in the configuration space, which is consequently of a higher dimension. *See also* STATISTICAL MECHANICS.

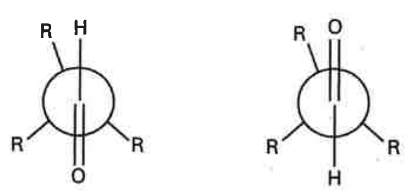
conformation One of the very large number of possible spatial arrangements of atoms that can be interconverted by rotation about a single bond in a molecule. In the case of ethane, $H_3C–CH_3$, one methyl group can rotate relative to the other. There are two extreme cases. In one, the C–H bonds on one group align with the C–H bonds on the other (as viewed along the C–C bond). This is an **eclipsed** conformation (or **eclipsing** conformation) and corresponds to a maximum in a



eclipsed conformation   anti conformation   gauche conformation

● = methyl group

Conformations of butane (sawhorse projection)



bisecting conformation   eclipsed conformation

Conformations of R_3CHO (Newman projection)

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