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Takeo Oku

SOLAR CELLS AND ENERGY MATERIALS

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Solar Cells and Energy Materials

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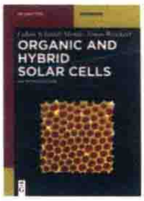

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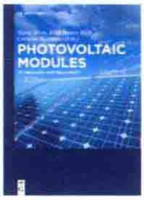

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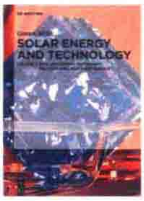

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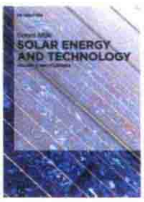

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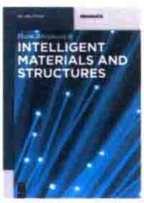

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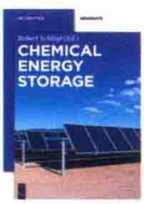

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Preface

"Let there be light". These words appear at the beginning of Genesis in the Old Testament. Advanced cosmological science has likewise shown that the universe started from a Big Bang 13.7 billion years ago. Light is an elemental root of our universe. The "flow of time" that we feel in what we perceive to be the present is an effect of the close relationship between light and matter, and time does not flow by itself. Quantum teleportation utilizing the connected spins of quantum particles at a distance results from principles that still remain unknown to contemporary scientists. Light has also not yet been entirely clarified by the advances of contemporary science, and several aspects of it remain unexplained.

On the other hand, light is essential to our everyday life in contemporary society. Light contains energy and information simultaneously, and most new electronic apparatuses, such as mobile phones, laptop computers, DVD players or satellite communications, function in ways closely connected to light.

After the big earthquake in Japan in 2011, all nuclear reactors in Japan were stopped, and some of them had already been closed previously. Saving electricity is promoted both in both industries and ordinary homes, and the world's energy problem has become a very familiar one in our everyday lives. Although Japan's energy self-sufficiency was 58 % in 1960, it had been significantly reduced to only 4 % by 2014. In other words, 96 % of the energy used in Japan depends on the import of materials such as oil, coal, liquefied natural gas and uranium, a fact that suggests improvements are needed to the current imbalance in supply and demand. Energy problems resulting from dependence on fossil fuels, which are limited energy resources, will soon be an inescapable issue all over the world. The author would be very pleased if the present book is helpful in solving future energy problems.

I would like to acknowledge many of my colleagues for their support, as follows: Atsushi Suzuki, Tsuyoshi Akiyama, Kenji Kikuchi, Taisuke Matsumoto, Akihiro Takeda, Akihiko Nagata, Kazuya Fujimoto, Junya Nakagawa, Hiroki Kidowaki, Nariaki Kakuta, Kazumi Yoshida, Masato Kanayama, Ryosuke Motoyoshi, Haruto Maruhashi, Masahito Zushi, Yuya Ohishi, Kohei Suzuki, Takuya Kitao, Taishi Iwata, Tatsuya Noma, Kazuma Kumada, Satoru Hori, Makoto Iwase, Yuma Imanishi, Yuji Ono, Kengo Kobayashi, Shiomi Kikuchi, Katsuhisa Tokumitsu, Mie Terada, Kouichi Hiramatsu, Masashi Yasuda, Yasuhiro Shirahata, Youichi Kanamori, Mikio Murozono, Yasuhiro Yamasaki, Mika Nakamura, Masahiro Yamada, Sakiko Fukunishi, Kazufumi Kohno, Misaki Fukaya, Yoshikazu Takeda, Akio Shimono, Eiji Ōsawa, Yasuhiko Hayashi, Tetsuo Soga, Tatsuo Oku, Ichihito Narita, Masaki Kuno, Naruhiro Koi, Atsushi Nishiwaki, Tadachika Nakayama, Katsuaki Suganuma and Brian D. Josephson. Thanks for excellent collaborative works, useful discussion, providing samples and experimental help. In addition, some figures were drawn after revision of original figures from some books and websites and I would like to offer my appreciation for

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November 2016, Takeo Oku

Table for physical constants

Physical constants	Symbol	Values	SI units
Velocity of light	c	2.99792458	10^{8} m s^{-1}
Planck constant	h	6.62607	10^{-34} J s
Dirac constant	$\hbar = h/2\pi$	1.05457	10^{-34} J s
Gravitational constant	G	6.67384	10^{-11} m^{3} s^{-2} kg^{-1}
Electron charge	e	1.60218	10^{-19} A s (C)
Electron mass	m_e, m_0	9.10938	10^{-31} kg
e Proton mass	m_p	1.67262	10^{-27} kg
Neutron mass	m_n	1.67493	10^{-27} kg
Electron energy	$m_e c^2$	0.5110	MeV
Compton wavelength	λ_c	2.4263	10^{-12} m
Boltzmann constant	k, k_B	1.38065	10^{-23} J K^{-1}
Magnetic permeability	$\mu_0 = 4\pi \times 10^{-7}$	1.25664	10^{-6} H m^{-1} (N A^{-2})
Dielectric constant	$\varepsilon_0 = 1/\mu_0 c^2$	8.85419	10^{-12} F m^{-1} (N V^{-2})
Avogadro constant	N_A	6.02214	10^{23} mol^{-1}
Gas constant	$R = k N_A$	8.31446	J K^{-1} mol^{-1}

Physical constants	Symbol	Values and units
Ångström	Å	0.1 nm = 10^{-10} m
Electron volt	eV	1.60218×10^{-19} J
Wavelength of 1 eV photon	λ	1239.84 nm
Standard atmosphere	atm	1.01325×10^{5} Pa

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Periodic table

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 H Hydrogen 1.008																	2 He Helium 4.003
3 Li Lithium 6.941	4 Be Beryllium 9.012											5 B Boron 10.81	6 C Carbon 12.01	7 N Nitrogen 14.01	8 O Oxygen 16.00	9 F Fluorine 19.00	10 Ne Neon 20.18
11 Na Sodium 22.99	12 Mg Magnesium 24.31											13 Al Aluminum 26.98	14 Si Silicon 28.09	15 P Phosphorus 30.97	16 S Sulfur 32.07	17 Cl Chlorine 35.45	18 Ar Argon 39.95
19 K Potassium 39.10	20 Ca Calcium 40.08	21 Sc Scandium 44.96	22 Ti Titanium 47.87	23 V Vanadium 50.94	24 Cr Chromium 52.00	25 Mn Manganese 54.94	26 Fe Iron 55.85	27 Co Cobalt 58.93	28 Ni Nickel 58.69	29 Cu Copper 63.55	30 Zn Zinc 65.41	31 Ga Gallium 69.72	32 Ge Germanium 72.64	33 As Arsenic 74.92	34 Se Selenium 78.96	35 Br Bromine 79.90	36 Kr Krypton 83.80
37 Rb Rubidium 85.47	38 Sr Strontium 87.62	39 Y Yttrium 88.91	40 Zr Zirconium 91.22	41 Nb Niobium 92.91	42 Mo Molybdenum 95.94	43 Tc Technetium (99)	44 Ru Ruthenium 101.1	45 Rh Rhodium 102.9	46 Pd Palladium 106.4	47 Ag Silver 107.9	48 Cd Cadmium 112.4	49 In Indium 114.8	50 Sn Tin 118.7	51 Sb Antimony 121.8	52 Te Tellurium 127.6	53 I Iodine 126.9	54 Xe Xenon 131.3
55 Cs Caesium 132.9	56 Ba Barium 137.3	57-71 Lutetium ♦	72 Hf Hafnium 178.5	73 Ta Tantalum 180.9	74 W Tungsten 183.8	75 Re Rhenium 186.2	76 Os Osmium 190.2	77 Ir Iridium 192.2	78 Pt Platinum 195.1	79 Au Gold 197.0	80 Hg Mercury 200.6	81 Tl Thallium 204.4	82 Pb Lead 207.2	83 Bi Bismuth 209.0	84 Po Polonium (210)	85 At Astatine (210)	86 Rn Radon (222)
87 Fr Francium (223)	88 Ra Radium (226)	89-103 Lawrencium ♦♦	104 Rf Rutherfordium (267)	105 Db Dubnium (268)	106 Sg Seaborgium (271)	107 Bh Bohrium (272)	108 Hs Hassium (277)	109 Mt Meitnerium (276)	110 Ds Darmstadtium (281)	111 Rg Roentgenium (280)	112 Cn Copernicium (285)	113 Nh Nihonium (284)	114 Fl Flerovium (289)	115 Mc Moscovium (288)	116 Lv Livermorium (293)	117 Ts Tennessine (294)	118 Og Oganesson (294)

Symbol for element →
Element →
Atomic mass (u) →

♦	57 La Lanthanum 138.9	58 Ce Cerium 140.1	59 Pr Praseodymium 140.9	60 Nd Neodymium 144.2	61 Pm Promethium (145)	62 Sm Samarium 150.4	63 Eu Europium 152.0	64 Gd Gadolinium 157.3	65 Tb Terbium 158.9	66 Dy Dysprosium 162.5	67 Ho Holmium 164.9	68 Er Erbium 167.3	69 Tm Thulium 168.9	70 Yb Ytterbium 173.0	71 Lu Lutetium 175.0
♦♦	89 Ac Actinium (227)	90 Th Thorium 232.0	91 Pa Protactinium 231.0	92 U Uranium 238.0	93 Np Neptunium (237)	94 Pu Plutonium (239)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (252)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (262)

Metal						Metalloid	Nonmetal			Unknown chemical properties
Alkali metal	Alkaline earth metal	Lanthanide	Actinide	Transition metal	Post-transition metal		Polyatomic nonmetal	Diatomic nonmetal	Noble gas	

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1 Energy

1.1 What is energy?

The word "energy" can have the following meanings:
1. The capacity for work that a certain system potentially has.
2. The ability to do physical work.
3. A useful resource for human society.
4. A resource required for physical or mental activity.

In the field of physics, energy generally refers to a quantity of work, as in definition (1). Heat, light, electromagnetic waves, and mass are also forms of energy. Within general usage, definitions (2) and (3) are more commonly used. There are many types of energy resources, and exhaustive energy and renewable energy have often been compared. Recently, a transition from exhaustive energy to renewable energy has begun taking place across the world.

The measurement used for energy in the International System of Units (SI unit) is the joule (J). The electron volt (eV) and kilowatt hour (kWh) are also used in the field of solar cells, as is shown in Table 1.1.

Table 1.1: Unit of energy.

Item	Symbol of quantity
Energy	E
Dimension	kg m^2 s^{-2}
Kind	scalar
SI unit	J (Joule)
CGS unit	erg = 10^{-7} J
MKS system of units	kgf m
Planck unit	Planck energy $E_P = 1.956\times 10^9$ J
Atomic unit	Hartree $E_h = 4.360\times 10^{-18}$ J
Kilo watt hour (kWh)	3.6 MJ
Electron volt (eV)	1.602×10^{-19} J

There are many types of energy, including: physical energy, kinetic energy, potential energy, elastic energy, chemical energy, ionization energy, heat energy, light energy, electric energy, acoustic energy, nuclear energy, mass energy and dark energy. Resources that are useful for industry, transportation and human life are generally referred to as "energy resources", which include oil, coal, natural gas, nuclear power energy, water power, solar heat and so on. Recently, a distinction has been made between energy resources that are exhaustive forms of energy and those that are re-

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newable. A development towards the increased use of renewable energy sources is currently in progress.

1.2 Fermions and bosons

An atom consists of a nucleus with positive charge and electrons with negative charge. The nucleus consists of protons with positive charge and electrically neutral neutrons. An electron is believed to be an elementary particle, and measures less than 10^{-18} m in diameter. Elementary particle is a general term for particles that cannot be further divided. Electrons do not orbit around the nucleus in the usual sense of the word, even though textbook figures often illustrate them as if they did. Electron clouds are stochastically distributed around the nucleus, which contributes to the size of the atom (diameter: ~ 0.2 nm). Electron clouds also exist like waves, which can be observed as a particle when measured. However, it is difficult to define the size of electron clouds. When atoms connect through chemical bonding to form molecules, or they are ionized, the size of atomic clouds change naturally and the size of atoms also becomes different.

The nucleus consists of protons and neutrons, and measures ~ 10^{-15} m (1 fm) in diameter. Mesons transmit the force of protons at a minute scale. According to the standard model, protons and neutrons consist of up and down quarks, and there are six types of quarks with three stages of generation in nature.

An electron is one of the six particles referred to as leptons. A proton consists of two up quarks and one down quark, and a neutron consists of one up quark and two down quarks, as shown in Fig. 1.1. These quarks are believed to be elementary particles at present, though superstring theory has also been proposed as a further

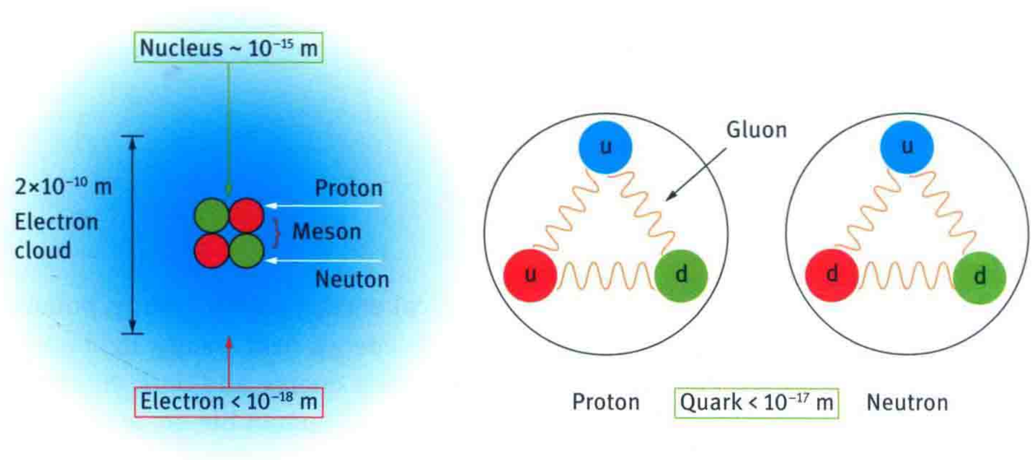

Fig. 1.1: Structure of atom, proton and neutron.

theory. Superstring theory indicates that elementary particles are a certain kind of string, and that quarks and leptons can be formed by the vibration of the strings. This theory is also called the quantum theory of gravity because of its inclusion of gravity.

Fermions are quantum particles with a spin angular momentum of half-integers such as 1/2, 3/2 and 5/2, as listed in Table 1.2. Fermions are guided by the Pauli Exclusion Principle, which indicates that two particles cannot occupy the same quantum state. Fermi-Dirac statistics apply to identical particles with half-integer spins in a system with thermodynamic equilibrium. The particles classified as fermions are quarks and leptons such as electrons, muons and neutrinos.

Table 1.2: Fermions and bosons.

Fermions	**First generation** Charge / Spin / Mass			**Second generation** Charge / Spin / Mass			**Third generation** Charge / Spin / Mass		
Quarks	Up u			Charm c			Top t		
	+2/3	+1/2	~ 2.3 MeV	+2/3	+1/2	~ 1.3 GeV	+2/3	+1/2	~ 173 GeV
	Down d			Strange s			Bottom b		
	−1/3	+1/2	~ 4.8 MeV	−1/3	+1/2	~ 95 MeV	−1/3	+1/2	~ 4.2 GeV
Leptons	Electron e^-			Muon μ^-			Tau τ^-		
	−1	+1/2	0.511 MeV	−1	+1/2	106 MeV	−1	+1/2	1.78 GeV
	Electron neutrino ν_e			Muon neutrino ν_μ			Tau neutrino ν_T		
	0	+1/2	< 2.2 eV	0	+1/2	< 170 keV	0	+1/2	< 16 MeV

Bosons	**Force**	**Charge**	**Spin**	**Mass**
Photon γ	Electromagnetic	0	1	0
Z boson Z^0	Weak	0	1	91.2 GeV
W boson $W^\pm$	Weak	± 1	1	80.4 GeV
Gluon g	Strong	0	1	0
Gaviton G	Gravty	0	2	0
Higgs boson H	Mass	0	0	126 GeV

On the other hand, bosons are quantum particles with an integer spin angular momentum, as listed in Table 1.2. A photon is a particle with a spin of 1. Bosons can occupy the same quantum state even in the case of more than one particle in one system. Bose-Einstein statistics apply to identical particles with an integer spin in systems with thermodynamic equilibrium. Examples of bosons include gauge particles, which carry the forces of elementary particles, such as photons, weak bosons and gluons. A graviton is an undiscovered boson with a spin of 2. A Higgs boson, which causes mass in elementary particles is a boson with a spin of 0. Cooper pairs, which are related to the phenomenon of superconductivity, obey Bose-Einstein statistics.

Neutrino is a general name for electrically neutral leptons, and neutrinos come in three flavors: electron neutrinos, muon neutrinos and tau neutrinos, associated with the electron, muon and tau, respectively. Although several quadrillion neutrinos pass through the human body each second, nobody feels them as they pass. Neutrinos almost never interact with matter, and it is quite difficult to observe them.

1.3 Important physical constants in the universe

The most important physical constants in our universe are the following:
- Velocity of light c (3.00×10^8 m s^{-1})
- Planck constant h (6.63×10^{-34} J s)
- Gravitational constant G (6.67×10^{-11} m^3 S^{-2} kg^{-1})

The Planck constant is a universal constant at the quantum scale. The energy of light (E) is proportional to the frequency (ν) of light, and the proportionality constant is a Planck constant.

$$E = h\nu \tag{1.1}$$

The velocity of light and the gravitational constant are large-scale constants valid across the universe, while the Planck constant is a constant at an extremely small scale.

1.4 Four fundamental forces of nature

- Gravity: The universal gravitation (F) between m_1 and m_2 at a distance of r is expressed as follows:

$$F = G\frac{m_1 m_2}{r^2} \tag{1.2}$$

Although gravitation interacts at a distance in a similar way to the electromagnetic force, gravitational force is very weak. Stars with high mass density attract and confine light, and can potentially form black holes.
- Electromagnetic force: The electrostatic force (F) between q_1 and q_2 with a distance of r is expressed by Coulomb's law as follows:

$$F = \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r^2} \tag{1.3}$$

ε_0 is a dielectric constant of a vacuum. Magnetic force functions similarly, and gravitational and electromagnetic forces depend on r^2. Various forms of energies central to life depend on the electromagnetic force, such as chemical reactions or bioenergy.

- Weak force: The weak force found by Fermi works at the elementary particle scale (10^{-18} m) and causes radioactive decay such as beta decay, in which a beta-ray (an electron) and an associated neutrino are emitted from an atomic nucleus.
- Strong force: The strong force is about 100 times stronger than electromagnetic force according to the theory of nucleus force and mesons. The interaction range of the strong force extends to about the size of nucleus (10^{-15} m) and its potential is expressed as follows:

$$U(r) \sim -\frac{g^2}{4\pi} \quad \frac{e^{-r/\lambda}}{r} \tag{1.4}$$

Where m is the mass of a meson, a particle has a Compton wavelength ($\lambda = h/mc$), and $g^2/4\pi$ is a bonding constant. As expressed by the exponential $e^{-r/\lambda}$, the force only acts at a close distance and other repulsive forces also act around the center of the nucleus.

These are the four forces that exist in the universe and their interaction ranges are different, as listed in Table 1.3. The forces interact through the distortion of fields and the exchange of particles. Gravitational and electromagnetic forces act over an infinite range. These four forces can be used in various ways as energy resources.

Table 1.3: The four fundamental forces as gauge bosons.

Particles mediating	**Photon** γ	**Weak boson** W, Z	**Gluon** g	**Graviton** G
Transmission force	Electromagnetic force	Weak force	Strong force	Gravitation
Strength scale ratio	10^{-2}	10^{-5}	1	10^{-40}
Spin	1	1	1	2
Mass	0	80, 91GeV	0	0
Acts on	Electric charge	Flavor	Color charge	Mass, energy
Functional ranges	Infinite	10^{-18} m	10^{-15} m	Infinite
Functional places	Atoms and molecules	Inside of nucleus	Inside of nucleus	Universal space
Energy source	Fossil fuels	Geothermal energy	Sun, nuclear energy	Hydropower, tide power