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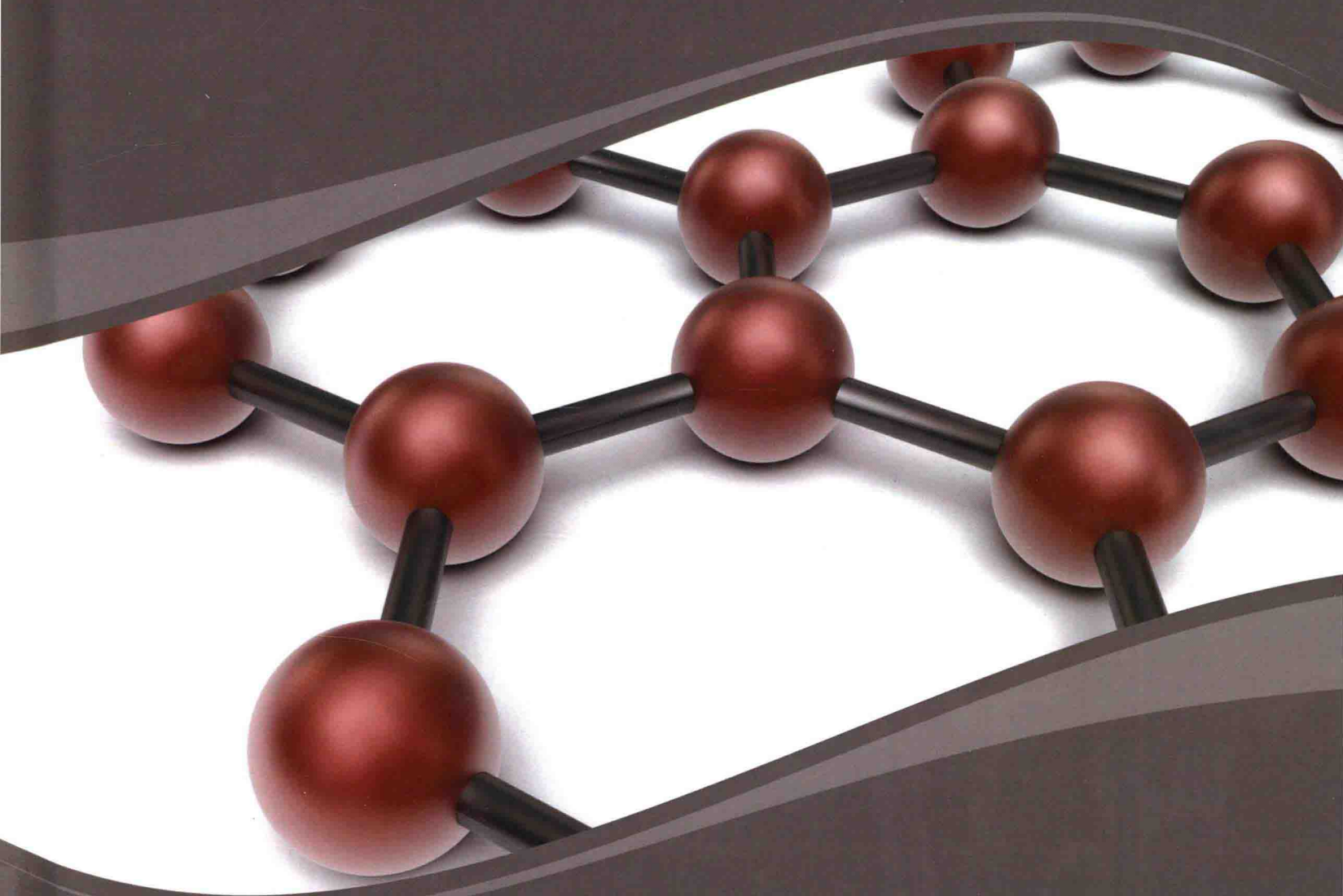

Mihai V. Putz

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Quantum and Optical Dynamics of Matter for Nanotechnology

Mihai V. Putz
West University of Timişoara, Romania

A volume in the Advances in Chemical and Materials Engineering (ACME) Book Series

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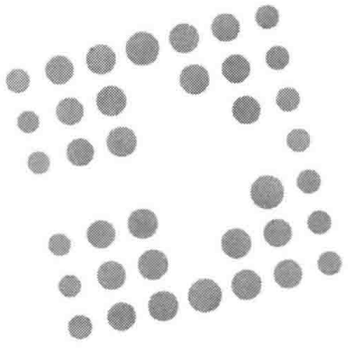

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Foreword

This book, with the broad range of covered topics, provides a comprehensive and instrumental treatise about the quantum theory foundation and description of the optical properties of (nano) matter, including non-linear optics and X-ray diffraction phenomena. The book offers modern and rich explanations of theoretical methods and experimental implications with agility in passing from one theme to another, which will positively surprise the interested reader.

The possible emergence, from the nanoscale realm, of a new physics, often related to low-dimensionality systems, is targeted by this volume whose primary audience remains professional theorists in material sciences, like physics, chemists, biochemists, and engineers. In addition, experimentalists and skilled students will find here very useful references for their studies.

The first of the book's three sections deals with quantum optics, introducing the mathematical basal instruments, which are required to fully understand the dynamic behaviors in quantum systems, including memory effect information, Markovian quantum master equation, molecular spectroscopy, and laser functioning. An extended theoretical description of non-linear optical effects completes the discussion. The second section begins by linking Ramsey mechanism with Raman optical sequences to present an exhaustive overview of atomic interferometry, accounting for the external gravitational contributions. Mathematical methods cover relevant topics like Einstein-Maxwell equations in dielectrics and gravitational influences imposed by General Relativity formalism on the pulse propagation.

The last section concludes the book with a detailed description of the physical principles underlying crystallographic measurements, which represent reliable experimental tools for nanostructure characterization in the presence of disorder. The presentation, by adopting both the geometrical and the dynamical models for X-ray diffraction, unveils the physical mechanisms driving X-ray propagation in a lattice and takes into account various important experimental applications like the fluorescence due to standing waves' anomalous absorption, asymmetrical Bragg factors, and inelastic diffraction phenomena.

Completeness and clarity are distinguishing characters of the author's scientific production.

I definitively think the reader will enjoy this book.

Ottorino Ori
Actinium Research, Rome

Ottorino Ori *was born in Soragna, Italy, in 1960. After the Italian master degree in theoretical solid state physics in 1986 (Parma University), he had a biannual post-doc position at Structural Chemistry departments in the same University of Parma funded by ENIRICERCHE, the research company of Italian oil company ENI, studying computer modeling of heterogeneous catalysis mechanisms in zeolitic systems. He was then with Thinking Machines Co., a Cambridge (US)-based company producing super computers mainly targeted for scientific applications. His marked interest for topologically based descriptors for chemical systems grew up in that environment, being the first scientist adopting topological invariants to characterize* C_{60}, C_{70} *and* C_{76} *fullerenes from 1992 on. Since 1996, his main professional interests have moved to industrial projects involving composites and nanomaterials mainly in the automotive and medical fields. He has published more than 40 papers in international scientific journals and is currently on the editorial boards of International Journal of Chemical Modeling (NOVA Pub) and Fullerenes, Nanotubes, and Carbon Nanostructures (Taylor & Francis).*

Preface

Since the 21st Century may be considered as belonging to nano-science and technology, the present book addresses in a concise advanced manner the quantum and optical dynamical properties of matter at nano-scale. The main quantum and optical concepts are reviewed and extended to properly characterize the atoms, molecules, and solids in their dynamic states. As such, the atomic absorption and interferometry, the molecular photo-dissociation and the dynamic X-ray diffraction on crystal structures, are discussed in depth, enabling the understanding of these complex processes of nature, in general, and of nano-tehnology, in particular.

Why is there a need for such a book? Without doubting the considerable value of the available books (some of them have been superior), they have not exhausted the scientific market of modeling the nano-system due to the increasing interest in this very broad field of fundamentals and applications; for instance, since this book is grounded in the author's student, researcher, and professor notes at/for lectures on spectroscopy, X-ray crystallography, and physical methods for chemistry and nanomaterials, the present endeavor adjusts and compiles the student taste for concise information, through compiling the available notions on a subject from various books and monographs, while having a few as the red line guide in the field, with the advanced research needs for a doctoral, post-doctoral, and confirmed researcher needs for having at his side the challenging problems and available and/or consecrated models in order to develop them further through feeling, intuition, and creativity. Therefore, the present textbook can be called a *concise advanced presentation*, being not too long with too much introductory material, while balancing between in depth quantum treatment of the subjects with specialized applications.

Accordingly, the present work is intended to present in an equilibrated manner the fundamental concepts and equations as well as of their combinations and applications in modeling complex natural or designed phenomena, stimulating the creative power of the reader interested not just in knowing-understanding but also in know-how predictions for the quantum information coined in the nano-scale systems by optical dynamics (e.g., as molecular photo-dissociations, atomic interference, and lattices' X-ray diffraction).

SECTION 1: QUANTUM DYNAMICS OF NANO-SYSTEMS

Chapter 1: *"Interacting Quantum Systems":* Basic quantum tools such as time-evolution operators, transition rates and amplitudes, statistical and projector operators, and interaction and density matrix representations are employed to characterize the open and interacting quantum systems with the aid of Schrödinger, quantum master, Fokker-Planck, and Feynman path integral equations and formulations.

Chapter 2: *"The Dynamics of Molecular Photo-Dissociation":* Quantum spectroscopy tools as absorption cross sections, autocorrelation functions, Fourier transformations, and Born-Oppenheimer approximations are employed for the phenomenological and analytical characterization of the molecular evolution under light interaction. Events such as photo-dissociation, photo-association, and molecular fragmentations with specialization to collinear triatomic molecular A+BC states are considered in this characterization.

Chapter 3: *"The Fundamentals of Quantum Optical Transitions":* Elementary and advanced concepts of quantum optics and spectroscopy are formulated, exemplified, and applied, and they relate the quantum states of a substance under electromagnetic action: from black-body radiation, to a spectral line profile's characterization by widths and intensities, to solving two-level spectral problems to understand the coherence and relaxation properties of light in matter.

Chapter 4: *"Light Amplification Analysis":* Main geometrical and quantum relationships between light and a substance are derived by characterizing the laser's light generation, threshold, resonances, stability, multimode locking and selection, polarization and stimulated Raman phase matching towards achieving the best energy gain, intensities, and optical information on the involved states either of light or of the substance that is investigated.

Chapter 5: *"The Basics of Non-Linear Optics":* Main analytical electromagnetic field theory tools were first used to describe the non-linear effects of light-light coupling as a basic cause of nonlinear optical phenomena and applications.

Chapter 6: *"Molecular Light Control in Rare-Gases Matrices – The HCl Case":* Various characteristics and mechanisms of HCl that has been entrapped in rare gas matrices (Ar, Kr, and Xe) are presented with regard to the spectroscopic characterization of exciplexes, cage exits, photo-dissociations, charge transfers, and the harpoonic mechanism. In addition, this chapter sheds light on specific quantum, potential, and reactive behavior of physical-chemical interactions.

SECTION 2: NANO-INTERFEROMETRY

Chapter 7: *"Raman Saturate Absorption":* Remarkable atomic population difference symmetry and coherence properties that are achieved without the custom laser-induced population inversion by the non-linear (Raman) saturated absorption spectroscopy are quantum mechanically explained and analytically modeled.

Chapter 8: *"Spectral Atomic Selection and Pumping":* Basic concepts of modern quantum optics as of Ramsey-Raman-Rabi spectroscopy through $\pi / 2 - \pi / 2$ pulses rather than by using a broad single light excitation of two-level atomic/molecular system towards atomic pumping, selection, and interferometer are exposed in an analytical and phenomenological manner.

Chapter 9: *"Gravitational Influence on Atomic Interference":* Two-level atomic systems are studied under gravitation influence and then employed in sequential pulse $\pi / 2 - \pi - \pi / 2$ towards modeling the Kasevich-Chu interferometer with matter waves.

Chapter 10: *"General Relativity Evolution of the Photons in Dielectrics":* Basic Einstein general relativity equations are linearized and coupled with Maxwell electromagnetic field equations to produce local gravitationally corrected Minkowsky space metrics; fundamental application on gravity action of an intense laser beam upon a weaker parallel one in dielectrics is undertaken towards evaluating of the space deviation phase shift and confirming the general equivalence principle of inertia for phonons in nanomaterials.

SECTION 3: NANO-DIFFRACTION

Chapter 11: *"General Concepts and Theories in X-Ray Diffraction":* The various forms of the X-Ray Diffraction (XRD) theory in the crystal are considered as perfect or imperfect for the version "perfect on portions" (i.e. with slight deformations or with a constant deformation gradient), following historical developments and performances of the models.

Chapter 12: *"Classical and Quantum Theories of Dynamic X-Ray Diffraction":* The main results of the dynamical theories of X-ray diffraction in their standard form of coupling of Maxwell equations with the Bloch waves on the one hand and the interaction of radiation-crystal in terms of perspective of quantum field on the other are unitarily presented.

Chapter 13: *"The Concept of X-Ray Standing Wave":* The concept of "Standing Waves" (SW) that arise in the crystal dynamically "attacked" by the frequency fields X is analytically analyzed towards expressing, in almost all the cases, the total intensity of the fields on dispersion branches in the perfect crystal and for the embedded layer on the imperfect crystal using various extensions of the semi-classical dynamic theory, adapted or reparameterized, depending on the specific conditions of analysis performed.

Chapter 14: *"Experimental Implications of X-Ray Standing Waves":* Basic concepts of dynamic X-ray diffraction are applied in distinguishing between the propagation along the atomic planes characterized by the linear absorption coefficient and the perpendicular propagation on the atomic planes. Propagation is responsible for the generation of the standing waves through the anomalous absorption coefficient on dispersion branches of diffraction.

Chapter 15: *"Absorption Coefficients of Inelastic Dynamic X-Ray Diffraction":* The X-ray inelastic scattering phenomena during the time-dependent perturbations are described with the aid of dynamical dispersion equations coupled with charge current in the Maxwell equations towards the appearance of the Debye-Waller factor driving the absorption coefficient, either for inelastic thermal diffusion and the Compton scattering, respectively.

Special features of the book are:

- Covers the optical effects of photo-dissociation, interferometry, and diffraction for complex matter nano-systems and the excited levels of molecules, atoms, and lattices, respectively;
- Covers non-linear optical phenomena;
- Includes detailed discussion of highly regarded optical transitions issue (whether quantum mechanically or semiclassically treated);
- Includes quantum characterization and set-up of lasers and of their optical output;
- Includes the general relativity treatment of matter's gravitation at nano-scale of atoms and photons;
- Presents the dynamical theory of X-ray diffraction in a concise and applied manner;
- Includes in the first section of the book special explicative and resumative tables such that the reader to can alternatively follow a kind of "short-intense" course on *laser spectroscopy* or to found further explanations and background as well having a "red line" with the main concepts and tools for going into the more advanced main text;
- References to some modern Web-available courses and theses in quantum optics.

Overall, the book complements the quantum and optics courses for graduation and master curricula of science and engineering physical chemistry, offering a modern equilibrated contents and fundamental tools for doctoral and post-doctoral studies as well, either at conceptual and analytical levels, while making systematic connection with experimental consequences and setups.

Certainly, since aware of the vast field of *photonics-based nanosciences*, as well by its importance in the years to come in science and technology, any constructive observations, corrections, and suggestions are welcome for providing a corrected, enlarged, and updated version of the present volume in its further editions; such peer contribution is welcomed.

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Section 1

Quantum Dynamics of Nano-Systems

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