MAGNETISM IN CARBON NANOSTRUCTURES

Magnetism in carbon nanostructures is a rapidly expanding field of current materials science. Its progress is driven by the wide range of actual and potential applications for magnetic carbon nanosystems, including transmission elements in spintronics, building blocks of cutting-edge nanobiotechnology, and qubits in quantum computing. These systems also provide novel paradigms for basic phenomena of quantum physics, and are thus of great interest for fundamental research.

This comprehensive survey emphasizes both the fundamental nature of the field, and its ground-breaking nanotechnological applications, providing a one-stop reference for both the principles and the practice of this emerging area. With equal relevance to physics, chemistry, engineering and materials science, senior undergraduate and graduate students in any of these subjects, as well as all those interested in novel nanomaterials, will gain an in-depth understanding of the field from this concise and self-contained volume.

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We may see how far from unproductive magnetick
philosophy is, how agreeable, how helpful, how divine!

William Gilbert, *De Magnete*, 1600

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Preface

Research on magnetic carbon nanostructures is a young and challenging field of materials science. It is in the process of widening our understanding of both items combined in the title of this book, of magnetism, and of carbon nanostructures. Magnetism in Carbon Nanostructures is taken here in the most general sense, which includes intrinsic magnetism as well as magnetism imported into a carbon nanostructure by a magnetic guest species. While effects of the latter type have been extensively studied, the former is the subject of lively current debate. It comprises a broad spectrum of magnetic phenomena not arising from conventional sources of magnetism in materials, i.e. the transition metals of the periodic table, but arising instead from structural irregularities, from dimensional reduction, defects and disorder. Equally persuasive as the promise of novel insight into the nature of magnetism and the basics of carbon nanostructures is the prospect of technological innovation offered by carbon-based magnetic materials. These materials are lighter than their metallic analogs. Also, they are expected to be available at lower fabrication cost and to be more efficient in terms of power consumption. In particular, during the past two decades, a wide range of actual and potential applications of carbon nanostructure magnetism have been identified, extending from fullerene-based magnetic resonance imaging (MRI) contrast agents to zigzag graphene nanoribbon (zGNR) transmission elements in nano-spintronics.

This text aims at a synoptic presentation of these advances, highlighting theory, experiment, and nanotechnological perspectives. Its main objective is to unite what is currently scattered over numerous articles in journals and conference proceedings, or found in individual chapters of multi-author monographs. Beyond these items, a great number of very instructive survey articles, illuminating various facets of carbon nanostructure magnetism, have been published. Likewise, excellent books on magnetism in condensed-matter systems or on carbon nanostructures (most notably on graphene, the topic of several extensive monographs that have appeared during the past few years) are available to readers, many of them covering some of the topics presented in this work. Yet, as far as I see, a comprehensive treatment of the subject, addressing the principles and the practice of carbon nanostructure magnetism in a single volume, is still lacking in this multitude of materials.

Therefore, I hope to satisfy with this publication a growing need of all those interested in novel nano-materials, be it as researchers or developers, as teachers or students. It is intended for a readership at the advanced undergraduate, as well as the graduate and the research level. Familiarity with quantum mechanics and thermodynamics at the level of the regular undergraduate curriculum in physics or chemistry is assumed. Due to the great variety of magnetic carbon nanostructures and, by the same token, the interdisciplinary nature of the field, a wide spectrum of different methods is used to study them. Naturally, this creates barriers that hinder communication between the practitioners of this field. For instance, an experimental chemist or materials scientist, specializing in magnetic metallofullerenes, and a theoretical physicist who explores magnetotransport through graphene, may be interested in each other's areas of expertise, but find it difficult to understand each other's language. Acknowledging this situation, I tried to make this book as self-contained as possible.

In accordance with this goal, I provide condensed introductions into the two principal concepts of this text, magnetism and carbon nanostructures. This material is covered in parts I and II of this book. The remaining three parts, dealing with intrinsic magnetism in carbon nanostructures, with magnetic transport phenomena, and with composite systems, contain the core material of this monograph.

Surveying a quickly expanding field of high current interest confronts the author with the task of hitting a rapidly moving target, a challenge compounded by the great diversity of the contributing science communities. Approaching the topic from various angles, those of physics, chemistry, and materials science, I attempted to provide a viable representation of the state of the art in the area of carbon nanostructure magnetism, but I did not strive to give maximum exposure to the most recent achievements in the field. While it was among my objectives to offer a snapshot of the current state of the field, I aimed still more at an organic presentation that develops, wherever possible, the tenets of carbon nanostructure magnetism from basic principles. Very recent proposals are included, but in some cases, the reader is referred to the relevant articles rather than taken through the often intricate details of what is not sufficiently assessed at this juncture. While I have aimed at a comprehensive survey that contains experimental and nanotechnological aspects, I am well aware that my own perspective, that of a computational physicist, shines through every page of the text.

Most chapters include some exercises which are intended to strengthen the reader's grasp of pertinent concepts, and also to bridge some gaps left in the main text. To avoid major digressions I have appended special-topic sections to some chapters. These supplements add background materials that are meant to aid understanding, or to highlight a theme of interest which nevertheless would block the flow of the narration if treated within the respective chapter. Some sections with additional content, intended to provide deeper or more detailed understanding, were not included in this volume to keep it at a manageable size. These portions are posted on my website: faculty.etsu.edu/HAGELBER/comp_chem.html

Those who have guided my efforts by sharing their knowledge on the topics of this book with me, or giving me insight into their own research, or supported me through words of criticism, or encouragement, or both, are too numerous to be listed here. My whole-hearted thanks go to all of them. I want, however, to acknowledge explictly those colleagues who worked with me on problems related to the subject of the book, namely Anahita Ayasoufi, Tandabany C. Dinadayalane, Oleksij V. Khavryuchenko, Danuta Lesczcynska, Jerzy Lesczcynski, Gilles H. Peslherbe, and, in the very first place, Jianhua Wu who first kindled my interest in carbon nanostructure magnetism and then became my tireless ally in exploring various facets of this field. I thank David Dixon, Jordan Gillenwater, Leo Memolo, and Dianna Pilkenton for immensely efficient help with preparing the figures reproduced in this volume. My gratitude goes to Karyn Bailey, Tessa de Roo, and Roísín Munnelly at Cambridge University Press for invaluable advice and assistance.

Authors tend to acknowledge their families for patiently enduring the great time demands associated with writing a book, and the author's reduced availability during that time. Far from merely tolerating the venture, my family was a constant source of support for me, inspiring in periods of progress, heartening in moments of despair. And so, my very special thanks go to my wife Elizabeth, and my children Ellen, Julia and Philip.