

Preface

The present book is dedicated to the theoretical modeling of nanostructures being the second one published on this topic in Springer Series *Nanoscience and Technology*.

The first book of this kind *Nanostructures: Theory and Modeling* was published in 2004 [1]. The authors of the book Prof. C. Delerue and Prof. M. Lannoo wrote in the preface that it is an introduction to the theory of nanostructures providing basic concepts for the physics of nano-objects and reviewing the theoretical methods of the nanostructure modeling. The authors have tried to make the book accessible to inexperienced readers, and it only requires basic knowledge in quantum mechanics and solid state physics.

Since 2004, the science of nanostructures has had an explosive growth [2]. The carbon nanotubes have remained to be widely investigated, including not only electronics and sensor technology, but also nanocatalysis and nanobiotechnology. The varied developments in carbon nanotubes are covered in book [2], citing over 2,000 references.

However, the nanostructures of a variety of inorganic materials have since been synthesized, their properties and applications have been investigated. In the book [2], the numbers of references cited are 500 and 900, respectively, in the case of inorganic nanotubes and nanowires.

An essential information about the structure and properties of inorganic nano-objects has been obtained due to the theoretical modeling and ab initio calculations of the nanostructure electronic properties. The use of the symmetry of one-periodic models of nanotubes and nanowires allows their calculations to be extended to the systems, consisting of 300–400 atoms.

The description of the symmetry and first principles treatment of the inorganic nanotubes based on BN, TiO_2 , and SrTiO_3 has been given by me recently in the chapter 13 of the book [3]. This book was published in 2012 as the second (enlarged) edition of my former book [4] in Springer Series in Solid State sciences, vol. 153. Since its online publication on January 18, 2013, there has been a total of 5,167 downloads for my book or its chapters on SpringerLink. This book was one of the top 25 % most downloaded eBooks in the relevant Springer eBook Collection in 2013.

I am sure that now it is time to cover the main results of the ab initio calculations made on the different inorganic nanostructures, describing in more detail their symmetry properties and overviewing the basic theoretical methods used, and the results obtained. This is the motivation of my book writing.

This book is divided in two parts.

Part I (Theory) of the book is intended for the experienced researchers who find in Chap. 2 the detailed description of the symmetry of the one-periodic (1D) nanotubes and nanowires. The basis of the modern ab initio methods of the nanostructure calculations is given in Chap. 3.

However, the book is also useful for the experimentalists who can omit the details of the ab initio methods description and read in Part II (Applications) the results of the theoretical modeling and ab initio calculations for the concrete inorganic nanostructures. To make such a work more convenient, I distributed the material in Part II over separate chapters in such a way that each chapter is dedicated to the concrete class of the inorganic nanostructures (boron compounds, tetravalent semiconductors, nitrides, oxides, sulfides).

Chaps. 4–6 in Part II include materials written by Prof. Yu. Zhukovskii (Institute of Solid State Physics, University of Latvia) and I am grateful to him for allowing me to use these materials in my book. He published a number of original papers on the ab initio treatment of inorganic nanostructures.

I am grateful to all my colleagues who took part in our joint nanostructure research (Prof. Yu. Zhukovskii, Dr. A. Panin, Dr. A. Bandura, Prof. D. Migas, Dr. S. Piskunov, D. Kuruch, M. Losev) or sent me fresh results of their research (Prof. M. Damnjanovic, Prof. P. Deak, Prof. R. Tenne, Dr. B. Aradi).

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