

Preface

Materials possess various properties such as magnetism, electric conductivity, ferroelectricity, photonics, thermal conductivity, mechanical properties, to name a few. In general, such properties do not alter independently of one another. Instead, strong couplings and interplay between these properties of materials can be noted. This is not surprising because various physical properties originate from the electronic structure of a material, i.e., a change in the electronic structure of a material will lead to changes in the physical properties of the material. Physical properties (usually representing functional aspects) can also be coupled with mechanical behaviors such as strain and deformation because a change in atomistic configuration brings about a change in electronic structure. The phenomena where multiple physical behaviors are intertwined is called ‘multiphysics’, which draws increasing interest due to its link to a wide range of possible applications such as strain engineering—which exploits the novel functions of devices by applying strain to them.

Multiphysics is significant and important in materials with nanostructures—nanometer-sized, low-dimensional materials such as ultrathin films, nanowires, nanoclusters, etc. Indeed, there has been a growing trend in fabricating nanodevices which utilize the interplay between the multiple properties of materials. The advent of first-principles calculation methods has been the driving force behind this trend because its methods enable highly accurate predictions of the properties and behaviors of nanostructures. The major drawback of first-principles calculations is surmountable due to the limited dimensions of the systems in question. There have been, therefore, a substantial number of theoretical studies, many of which have been based on first-principles calculation methods, to acquire an in-depth understanding and knowledge about ‘multiphysics in nanostructures’, this trend is expected to gain even more momentum in the following years and decades.

The purpose of this book is to systematically review recent advances in the theoretical investigations of the multiphysics phenomena in nanostructured materials by introducing a wide variety of studies including elastic strain engineering. This book mainly covers broad topics on the remarkable properties of multiphysics in low-dimensional nanoscale components, investigated by means of first-principles density functional theory. The book also includes studies based on semi-empirical

electronic structure calculations such as the tight-binding method. These methods help us understand the complicated nature of non-linear multiphysics couplings due to quantum mechanical effects. We believe that this book serves as motivation for readers to explore the rapidly expanding world of multiphysics in nanostructures, which itself paves the way for exploiting and designing novel functionalities at the nanoscale. We hope readers will be interested in this exciting multidisciplinary field and will be motivated to get involved in this promising research area.

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