

Preface

The field of nanomaterials has become one of the most quickly growing areas in science due to the unique properties and potential applications of these materials in electronics, medicine, consumer goods, defence, amongst others. Nanomaterials come in different shapes including zero-dimensional (0D), one-dimensional (1D) and two-dimensional (2D) forms. They are classified by having at least one of their dimensions less than 100 nm in size.

The class of 2D nanomaterials are characterised by large lateral dimensions and small thicknesses of the order of less than, typically, several nanometres. They are often referred to as nanosheets and can be considered akin to extremely thin sheets of paper. A wide variety of materials can be grown as 2D nanomaterials and can be composed of one or multiple elements. The elemental 2D nanomaterials usually have names ending in 'ene' and include the material that is the focus of this book, namely silicene. Silicene is a crystalline two-dimensional (2D) nanomaterial composed entirely of silicon (Si) atoms. The atoms in this single layer are arranged in a hexagonal honeycomb structure which, when viewed from the side, are buckled.

Other 2D elemental nanomaterials include the well-known structure graphene (composed of carbon), as well as phosphorene (composed of P), germanene (composed of Ge) and stanene (composed of Sn). There are also 2D nanomaterials composed of different compounds (usually consisting of two elements covalently bonded together). Examples include the transition metal di-chalcogenides having the composition of MX_2 , with M being a transition metal atom (Mo, W, etc.) and X a chalcogen atom (S, Se or Te). Common examples include MoS_2 , WS_2 , $MoSe_2$, WSe_2 and $MoTe_2$.

This book is dedicated to discussing the structure, properties and applications of silicene. While there are a number of excellent review articles that have been published on this material, we have brought together top scientist working on different aspects of silicene to provide a state-of-the-art and up-to-date account of a wide variety of aspects of the material.

At the time of publication of this book >700 papers have been published on silicene (based on a search of Web of Science using the term ‘silicene’). More than 450 of these were published in 2014 and 2015 alone. Of course, this does not find all articles published on this material, particular the early work performed in the area before the term silicene was used or recognised. Indeed, some of our early papers used the term ‘Si nanosheets’ to refer to multilayer or functionalised silicene. The numbers, however, do give an indication of the popularity of the material and how fast the field is growing.

The name silicene was first coined by G.G. Guzman-Verri and L.C. Lew Yan Voon in 2007 in their paper on the electronic structure of silicon-based nanostructures in *Physical Review B*. Thicker variants of silicene are referred to as nanosheets, or more recently, multilayer silicene.

Silicene has been studied using a variety of methods including different experimental techniques as well as different theoretical or computational approaches. The information provided by the different techniques has helped to generate complementary information to advance our understanding of this material.

This book is divided into 3 sections. The first section of the book (Part I) is dedicated to unmodified free-standing silicene and multilayer silicene. Chapter 1 discusses the physical properties of free-standing silicene, including its structure, mechanical, electronic, electric field, topological, optical, transport, magnetic and thermal properties. A brief discussion on defects and doping is also included. As silicene has not been synthesised unmodified in the free-standing form, the results are primarily theoretical in nature. Chapter 2 reviews the topological properties of 2D elemental honeycomb nanosheets of the Group 14 elements, which includes silicene. Chapter 3 discusses the formation, structural and electronic properties of unmodified free-standing multilayer silicene that has been studied using molecular dynamics and density functional theory (DFT) approaches.

The second section of the book (Part II) reviews the properties of silicene that are modified by molecular chemisorption or when interfaced with non-metallic surfaces. Specifically, Chap. 4 discusses the soft chemical synthesis of silicene functionalised with different chemical groups and the potential applications of such materials. Chapter 5 reviews the theoretical studies and in particular the DFT calculations of functionalised silicene and the associated structural, electronic and dynamic properties. Chapter 6 covers theoretical work examining the interaction between silicene and non-metallic surfaces such as aluminium nitride, layered metal (di)chalcogenides, ZnS surfaces as well as possible growth of silicene on MoS₂. The findings are compared to experimental results where available.

The third section of the book (Part III) covers the studies of silicene on different substrates and presents both the theoretical and experimental results. There is a significant body of work that has focused on the deposition of silicene onto single crystal silver (Ag) surfaces and we dedicate Chaps. 7–12 to the different aspects of work in this area. In Chap. 7, the experimental studies of silicene grown on the Ag (111) single crystal surface are reviewed. There are many different overlays that form on this surface and the structures and their associated electronic properties are presented. Chapter 8 covers the growth of silicene on the Ag(111) and Au(110)

surfaces. While there is some overlap with Chap. 7 we believe that this is warranted due to the volume of work in this area, and in particular, the inclusion of multilayer silicene on the Ag(111) surface is emphasised. Chapter 9 discusses the growth of silicon nanoribbons on the Ag(110) surface. While we have mainly focused the book on extended silicene, we believe that having a chapter focused on nanoribbons (similar to strips, or ‘ribbons’ of silicene) will be of interest to the reader, as there is a school of thought as to whether the nanoribbons can actually be distinguished from pure silicene. Chapter 10 gives a comprehensive review of the theoretical studies of silicene on different silver surfaces. Chapter 11 presents work on the adsorption and interaction of different molecules on silicene. This aspect of the field is particularly important for determining the potential application of silicene in nanoelectronics or other devices, where they need to operate under environmental conditions. Chapter 12 concludes the book with a review of the studies that have examined deposition of silicene on substrates other than silver and include several conductive substrates such as $\text{ZrB}_2(0001)$, $\text{ZrC}(111)$, $\text{Ir}(111)$ and $\text{Au}(110)$, in particular.

As editors and authors of this book, we are very pleased to have been involved in publishing what we believe is the first book wholly dedicated to this exciting new material. The chapters presented here will provide a solid foundation for those starting out in the field, including undergraduate and postgraduate students studying chemistry, physics, engineering and nanotechnology. For the experts already working on silicene and 2D nanomaterials as experimentalists and/or theoreticians, we believe that this will provide a source of invaluable information and a useful reference.

Of course, the work on silicene is still a growing area of research and there are many questions yet to be answered about the potential of this material. We are very excited to be part of the discoveries in this area and look forward to seeing where this material will go in the future. We hope that you as the reader will share in our passion for science and 2D nanomaterials!

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Silicene

Structure, Properties and Applications

Spencer, M.; Morishita, T. (Eds.)

2016, XVI, 276 p. 149 illus., 102 illus. in color.,

Hardcover

ISBN: 978-3-319-28342-5