Solid State Materials Chemistry

This book explores the fascinating world of functional materials from the perspective of those who are tasked with inventing them, solid state chemists. Written in a clear and accessible style, this book provides a modern-day treatment of solid state materials chemistry for graduate and advanced undergraduate level courses. With over 330 problems and 400 original figures, this essential reference covers a wide range of materials in a holistic manner, including inorganic and organic, crystalline and amorphous, bulk and nanocrystals.

The introductory chapters cover topics such as crystal structures, defects, diffusion in solids, chemical bonding, and electronic band structure. Later chapters focus on important classes of functional materials including pigments, phosphors, dielectric materials, magnets, metals, semiconductors, superconductors, nonlinear optical materials, battery materials, zeolites, metal–organic framework materials, and glasses. The technological applications and synthesis methods used to prepare the materials that drive modern society are highlighted throughout.

Patrick M. Woodward is a Professor in the Department of Chemistry and Biochemistry and holds a courtesy appointment in the Department of Physics at Ohio State University. He is best known for his studies of the structures and properties of perovskite-related materials. He has served as chair of the Solid State Chemistry Gordon Conference (2018), Associate Editor of the *Journal of Solid State Chemistry* (2006–2011), and Vice President of the Neutron Scattering Society of America (2014–2018). He is co-author of the widely used general chemistry textbook, *Chemistry: The Central Science* (Pearson Education Limited, 2018). Patrick is a recipient of an NSF Career Award (2001), a Sloan Research Fellowship (2004), a Leverhulme Visiting Professorship (2017), and is a Fellow of the American Chemical Society (2020).

Pavel Karen is a Professor in the Department of Chemistry at the University of Oslo. His interests include inorganic reaction chemistry, solid state synthesis methods, crystallography, phase relations and thermodynamics, and point-defect chemistry; all components of his teaching portfolio. He is interested in the relationship between structure and properties of less common inorganic solids, such as mixed-valence oxides. Crystal structures are studied by X-ray and neutron diffraction, local structures by Mössbauer spectroscopy, and valence-mixing by calorimetry. He is co-author of the chapter Phase Diagrams and Thermodynamic Properties in the *Handbook on the Physics and Chemistry of the Rare Earths, Volume 30, High-Temperature Superconductors* (Elsevier, 2000). Pavel is a member of the American Chemical Society, the American Crystallographic Association, and of the International

Union of Pure and Applied Chemistry's Division II and the Interdivisional Committee on Terminology, Nomenclature and Symbols.

John S. O. Evans is a Chemistry Professor at Durham University where he served as Head of Chemistry from 2009 to 2014. His research interests are in the synthesis and properties of (mainly) inorganic materials, their structural chemistry, and their real-world applications. In recent years he has worked, inter alia, on negative thermal expansion, symmetry properties of phase transitions, new oxide-chalcogenides and energy-related materials. He has a long-standing interest in developing powder diffraction methods and is co-author of *Rietveld Refinement: Practical Powder Diffraction Pattern Analysis using TOPAS* (De Gruyter, 2019). John was awarded the 1997 Meldola prize of the Royal Society of Chemistry, and was co-awarded the 2015 Royal Society of Chemistry Teamwork in Innovation Award for work with industry.

Thomas Vogt is the Educational Foundation Endowed Chair in the Department of Chemistry and Biochemistry, Director of the NanoCenter and adjunct Professor in the Department of Philosophy at the University of South Carolina. His work focuses on establishing structure–property relationships of solid state materials using X-ray and neutron scattering and electron microscopy. He is recognized as Fellow of the American Physical Society, the American Association for the Advancement of Science, the Institute of Advanced Study at Durham University, and the Neutron Scattering Society of America. Thomas received the Carolina Trustee Professorship of the Board of Trustees in 2018 as well as the University of South Carolina's Educational Foundation Award for Research in Science, Mathematics, and Engineering in 2019.

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Patrick M. Woodward
Ohio State University

Pavel Karen
Universitetet i Oslo

John S. O. Evans
Durham University

Thomas Vogt
University of South Carolina

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Preface

Functional materials are an integral part of daily life. As an example, consider the materials that underpin smartphone technology. The integrated circuitry is made from complex patterns of semiconductors, metallic conductors, and insulators. Organic light-emitting diodes convert electrical signals from the processor into a vibrant high-resolution color display. The display is protected by a screen made from tough but lightweight Gorilla® glass, which is coated with a transparent conducting oxide to make the screen responsive to the touch of a finger. Magnetic materials are used in the speakers, a lithium-ion battery powers the device, specific dielectric materials are used to receive and isolate a call once the signal reaches a base station, and the list goes on.

This book explores the fascinating world of functional materials from the perspective of those who are tasked with inventing them, solid state chemists. We therefore adopt the chemist's definition of a material as a substance whose structure and properties are controlled at the atomic level to produce a specific function. Returning to our example, a modern smartphone contains over half of the non-radioactive elements on the periodic table. A few are used in their elemental form, but in most cases the desired function can only be achieved by combining elements to form compounds. With the periodic table as a palette, how does the chemist design and synthesize the mind-boggling variety of functional materials that future technologies depend upon? That question is the topic this book explores.

The book is written specifically with teaching in mind and is intended primarily for use in upper-level undergraduate or graduate level courses. While our perspective is that of a chemist, the book is accessible to physicists and engineers as well. Mathematical details are given where they add deeper understanding, but the focus is always on relating the properties of a material to the characteristics of the atoms and molecules from which it is built.

The first six chapters cover the fundamentals of extended solids: crystal structures, defects, reactivity, phase diagrams, phase transitions, chemical bonding, and band structure. The remaining chapters, each of which is organized around a specific property or class of materials, show how the properties of modern functional materials can be understood from these fundamental concepts. Recognizing that the field of solid state chemistry is much more expansive than can be covered in a single course, the later chapters are designed to be largely independent of each other. This organization provides the instructor freedom to tailor a course to cover those materials that are most relevant for their students.

Coverage of inorganic and organic materials is interwoven throughout the book to place the emphasis on properties. To keep the scope at a manageable level, neither synthesis nor

characterization are covered in detail. Instead, boxes on synthetic methods and characterization methods are placed throughout the book to highlight specific examples. In a similar vein, boxes are used to describe how the properties of nanoscale solids differ from bulk materials (Nanoscale Concepts), and to highlight important technological applications of materials (Materials Spotlight). Students learn by practice, and, in this spirit, we have included dozens of problems at the end of each chapter to allow students to test their understanding of the concepts covered in the chapter. Instructors can obtain a full set of worked solutions on request.

We hope that this book will be a valuable source of learning for the next generations of solid state scientists and engineers and a resource for those who already work in this fascinating field.

Patrick Woodward
Pavel Karen
John Evans
Thomas Vogt

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