Preface

This special edition presents a collection of studies dedicated to the computational modelling, simulation, and functional properties analysis of advanced materials across various engineering domains and scientific research. The contributions illustrate how computational tools, numerical methods, and theoretical approaches contribute to materials design, their processing optimisation, and performance evaluation.

Chapter 1: Computational Materials Physics provides insight into the fundamental principles and simulation methods used to predict and analyse material properties at the atomic and electronic scales. It highlights how computational physics contributes to understanding material behaviour and control of experimental research.

Chapter 2: Numerical Study of Structural Materials and Technologies focuses on modelling and numerical analysis of engineering materials' mechanical and physical behaviour. The chapter discusses computational techniques that support developing and optimising structural components and technologies under diverse operating conditions.

Chapter 3: Modelling Particle Behaviour in Technological Flow explores the dynamics of particles in various flow systems, addressing challenges related to fluid–solid interactions, multiphase processes, and transport phenomena.

Chapter 4: Materials for Biomedical Applications examines materials' properties and functionality in biomedicine. It observes the issues of biocompatibility, functional effectiveness, and material–tissue interactions that contribute to the development of modern medications and therapeutic procedures.

The special edition aims to serve as a valuable reference for researchers, engineers, and students engaged in computational materials science, applied physics, and engineering technologies.