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"*This timely book highlights the state of the art in computational approaches currently being investigated to predict nanomaterial toxicity and support safety by design. It is a must-read for all those involved in computational nanotoxicology research as well as those working in industry or regulatory bodies who seek to understand how these approaches could be used to support safety-by-design nanotechnology.*"

Dr. Richard L. Marchese Robinson
University of Leeds, UK

The development of computational methods that support human health and environmental risk assessment of engineered nanomaterials (ENMs) has attracted great interest because the application of these methods enables us to fill existing experimental data gaps. However, considering the high degree of complexity and multifunctionality of ENMs, computational methods originally developed for regular chemicals cannot always be applied explicitly in nanotoxicology. This book discusses the current state of the art and future needs in the development of computational modeling techniques for nanotoxicology. It focuses on (i) computational chemistry (quantum mechanics, semi-empirical methods, density functional theory, molecular mechanics, molecular dynamics), (ii) nanochemoinformatic methods (quantitative structure–activity relationship modeling, grouping, read-across), and (iii) nanobioinformatic methods (genomics, transcriptomics, proteomics, metabolomics). It reviews methods of calculating molecular descriptors sufficient to characterize the structure of nanoparticles, specifies recent trends in the validation of computational methods, and discusses ways to cope with the uncertainty of predictions. In addition, it highlights the status quo and further challenges in the application of computational methods in regulation (e.g., REACH, OECD) and in industry for product development and optimization and the future directions for increasing acceptance of computational modeling for nanotoxicology.

Agnieszka Gajewicz is assistant professor at the University of Gdansk, Poland. She has authored more than 45 research publications in leading nanotechnology- and environment-related journals and has received prestigious international and national awards, including the L'Oréal-UNESCO International Rising Talents Award For Women in Science and a fellowship of the Polish Minister of Science and Higher Education for outstanding young researchers. Her current research interests include the development and application of machine learning, statistical learning theory, and chemometrics to address problems and challenges in computer-based methods for chemical safety assessment and the design of new chemicals (nanomaterials, ionic liquids) that are safe for human health and the environment.

Tomasz Puzyn is professor at the Laboratory of Environmental Chemometrics, Faculty of Chemistry, University of Gdansk, Poland. He has authored more than 120 research papers in leading nanotechnology- and environment-related journals and edited 4 books. His main achievement is the introduction of quantitative structure–activity relationship (QSAR) modeling in nanotechnology. He has led two completed EU FP7 projects and participated in five H2020 projects conducted within the European NanoSafety Cluster. He has received prestigious national and international awards, including fellowships of the Japan Society for the Promotion of Science, the Foundation for Polish Science, and the Polish Minister of Science and Higher Education. Prof. Puzyn is founder and CEO of QSAR Lab Ltd., a spin-off company that uses the potential and experience of research staff from the Laboratory of Environmental Chemometrics to support chemical, cosmetic, and pharmaceutical industries in developing computational methods for designing innovative products (nanomaterials, ionic liquids) that are safe for humans and the environment.

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