

# Preface

With a great pleasure, we take this opportunity to bring the current volume “Energetic Materials: From Cradle to Grave” under the series “Challenges and Advances in Computational Chemistry and Physics”. This volume brings experimentalists and theoreticians on a common platform integrating recent advances in the “Cradle to Grave” of munition compounds through scholarly contributions. The 13 contributed chapters included in this volume cover wide area ranging from design and development of munitions, nanomaterials in munitions application, fate and transport, and munition-induced toxicity.

Chapter “[High Performance, Low Sensitivity: The Impossible \(or Possible\) Dream?](#)” contributed by Politzer and Murray discusses the design and development of high-performance and low-sensitivity munitions (insensitive munitions), their characteristics, and how and if such dream can be materialized. Chapter “[Recent Advances in Gun Propellant Development: From Molecules to Materials](#)” by Rozumov provides an overview of recent advances in the development of gun propellants including making the gun propellant formulations less sensitive to shock and thermal stimuli. The utilization of quantitative structure–property relationships (QSPR) models in the design and development of munition compounds including prediction of various properties has been the focus of the next chapter by Fayet and Rotureau. The use of energetic polymers is expected to be beneficial since they contribute several advantageous characteristics such as temperature and pressure stabilities, produce less smoke, and so on. The recent advances in the synthesis and applications of energy polymers have been reviewed by Paraskos in Chapter “[Energetic Polymers: Synthesis and Applications](#)”. The large surface area and enhanced reactivity of nanoscale metallic powder can be utilized as an efficient pyrophoric materials. In Chapter “[Pyrophoric Nanomaterials](#)”, Haines et al. present an overview of recent progress in pyrophoric nanomaterials including pyrophoric foams and various safety consideration.

In the rocket motor design, the information about the burning rate of propellant plays an important role. Isert and Son have reviewed the relationship between flame structure and burning rate for ammonium perchlorate composite propellants in Chapter “[The Relationship Between Flame Structure and Burning Rate for Ammonium](#)

[Perchlorate Composite Propellants](#)". Picatinny Arsenal FRAGmentation (PAFRAG) is used to evaluate explosive fragmentation ammunition lethality and safe separation distance without costly arena fragmentation tests. The fundamentals of this methodology and applications have been reviewed in the next chapter by Gold. In Chapter ["Grain-Scale Simulation of Shock Initiation in Composite High Explosives"](#), Austin et al. have detailed the application of single- and multi-crystal simulation to understand response and detailed chemical and physical processes for energetic material safety. In the next chapter, Mukherjee and Davari have reviewed the development of various computational models to investigate fate, transport, and evolution of energetic nanomaterials. In Chapter ["Physical Properties of Select Explosive Components for Assessing Their Fate and Transport in the Environment"](#), Boddu et al. have reviewed the physical properties for assessing the fate and transport of select munition compounds in the environment. In Chapter ["High Explosives and Propellants Energetics: Their Dissolution and Fate in Soils"](#), Dontsova and Taylor have reviewed the dissolution and fate of high explosives and propellants in soils while in the following chapter, Taylor et al. have reviewed the fate and dissolution of insensitive munitions formulations in the soils. The last chapter by Lotufo provides a comprehensive overview of toxicity and bioaccumulation of energetic compounds in the aquatic and soil organisms and in terrestrial plants.

We take this opportunity to thank all contributors for devoting their time and hard work to make this project a success. We would like to thank Dr. Elizabeth A. Ferguson, Senior Science Technical Manager and Lead Technical Director for Environmental Quality and Installations, US Army Engineer Research and Development Center, Vicksburg, Mississippi, USA, for continuous support and encouragement to publish this book. Of course, many thanks go to our family members and friends. Without their support, the development and completion of the book would not have been possible.

Vicksburg, MS, USA  
Peoria, IL, USA  
Vicksburg, MS, USA  
Picatinny, NJ, USA  
Jackson, MS, USA

Manoj K. Shukla  
Veera M. Boddu  
Jeffery A. Steevens  
Reddy Damavarapu  
Jerzy Leszczynski

Energetic Materials

From Cradle to Grave

Shukla, M.; Boddu, V.M.; Steevens, J.A.; Damavarapu, R.;  
Leszczynski, J. (Eds.)

2017, VIII, 482 p. 191 illus., 49 illus. in color., Hardcover

ISBN: 978-3-319-59206-0