Editorial

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Revolutionizing Energetic Materials Discovery and Design: The Role of Data Science and Machine Learning

This Special Issue of Propellants, Explosives, Pyrotechnics (PEP) is focused on energetic materials discovery and design using Data Science and Machine Learning (DS&ML). The application of DS&ML has proven to be transformative in many areas, where it has been shown to expedite analysis, enable extraction of greater quantities of information from datasets, and guide experiments. However, energetic materials and their applications present unique challenges that often hinder the use of standardized tools and practices. In spite of these challenges, important and compelling advancements are being made toward data-directed research in energetics.

We seek to accomplish four things in this issue: (1) provide the PEP audience with an opportunity to learn how their work can benefit from DS&ML, (2) serve as a starting point for collaborations and conversations on how DS&ML can be applied to areas of interest to PEP readership, (3) provide concrete examples of successful applications of DS&ML that have been applied to propellants, explosive and pyrotechnics, and (4) highlight experimental techniques conducive to post-processing or on-the-fly analysis using DS&ML.

Energetic materials play a crucial role in a broad array of applications. Developing new energetic materials with improved properties such as higher energy-density compounds with greater power output, improved stability, and lower sensitivity to external stimuli is an ongoing scientific challenge. One technical barrier to progress in these areas are that energetic materials can be highly unpredictable, where their behavior can change dramatically in response to factors such as subtle changes in temperature, pressure, and aging. This unpredictability has traditionally made it difficult to design and test new materials efficiently, and hence leads to costly trial and error processes. It is apparent that the area of energetic materials discovery and development can benefit greatly with shifts toward using DS&ML approaches to accelerate the scientific, engineering and manufacturing progress.

The advantage of using DS&ML in energetic materials discovery is not just limited to the ability to process and analyze large datasets quickly but also to help better identify cause and effect relationships. For instance, DS&ML methods can enable researchers to identify patterns and correlations in data that may not be immediately apparent when using traditional approaches. By leveraging these insights, researchers can develop more accurate models for predicting material structure-property-performance relationships of new materials with that added benefit of significant reductions in the time and resources required for their design and development. Another attribute of using DS&ML in energetic materials discovery is the ability to explore new chemical spaces. Traditional experimental methods can be limited by the number of possible chemical combinations that can be synthesized and tested. In contrast, DS&ML can explore much larger chemical spaces, enabling researchers to identify promising new materials that may have been overlooked using traditional methods.

While there is no doubt that DS&ML has the potential to revolutionize the field of energetic materials discovery and development there are challenges that need to be addressed. One of the most significant challenges is the lack of high-quality and/or extensive data available for training DS&ML models.

In conclusion, DS&ML techniques have the potential to accelerate the discovery and optimization of new energetic materials. While there are challenges that need to be addressed, the continued development and application of these techniques is likely to have a significant impact on the area of energetic material discovery and development in the coming years.

We believe this Special Issue will provide PEP readers with an excellent overview of DS&ML applied to the area of energetics. The editors of PEP are grateful to the authors of the contributed papers.

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