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A perspective on modeling the multiscale response of energetic materials

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The response of an energetic material to insult is perhaps one of the most difficult processes to model due to concurrent chemical and physical phenomena occurring over scales ranging from atomistic to continuum. Unraveling the interdependencies of these complex processes across the scales through modeling can be done only within a multiscale framework. In this talk, I will describe our philosophy and progress in the development of a predictive, experimentally validated multiscale reactive modeling capability for energetic materials. I will also describe new opportunities and challenges that have arisen in the course of our development that will be pursued in the future.