

Abstract for an Invited Paper
for the SHOCK11 Meeting of
The American Physical Society

Multiscale Modeling of Energetic Materials: Easy to Say, Harder to Do

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In recent years, multiscale modeling has routinely been included in materials research programs (including those involving energetic materials). However, too often multiscale modeling is applied in a piecemeal fashion due to the fledgling state of multiscale modeling. While the concept of multiscale modeling of energetic materials is straightforward, practical implementation of this type of hierarchical modeling is hindered by numerous technical challenges. This talk reports on our efforts in establishing a multiscale modeling capability to predict energetic material response and includes a discussion of emerging models, methods and software, stumbling blocks, and lessons learned in this new area of exploration within our laboratory.