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Analyzing and Predicting the CL-20 Detonation Reaction Mechanism Based on Artificial Intelligence Algorithm

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Abstract : In order to solve the problem of a large amount of simulation and limited simulation scale in the first-principle molecular dynamics simulation of energetic material detonation reaction, we established an artificial intelligence model for analyzing and predicting the detonation reaction mechanism of CL-20 based on the first-principle molecular dynamics simulation of the multiscale shock technique (MSST). We employed principal component analysis to identify the dominant charge features governing molecular reactions. We adopted the K-means clustering algorithm to cluster the reaction paths and screen out the key reactions. We introduced the neural network algorithm to construct the mapping relationship between the charge characteristics of the molecular structure and the key reaction characteristics so as to establish a calculation method for predicting detonation reactions based on the charge characteristics of CL-20 and realize the rapid analysis of the reaction mechanism of energetic materials.

Keywords : energetic material detonation reaction, first-principle molecular dynamics simulation of multiscale shock technique, neural network, CL-20
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