

Abstract Submitted
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Density functional theory study of CeD_x with application to ejecta break-up in reactive gases JOSIAH BJORGAARD, DANIEL SHEPPARD, Los Alamos Natl Lab — When ejecta are produced in a reactive gas, the diffusion of the reacting gas into the ejecta particles may have an important effect on break-up. This can influence the rate of break-up, particle size, and composition. In this study, density functional theory calculations were performed to explore the properties of CeD_x in support of experiments of Ce ejected into D gas. Under these conditions, the diffusion of D into Ce ejecta is of fundamental importance to the ejecta physics. We perform quantum molecular dynamics simulations to derive fundamental quantities including temperature dependent diffusion coefficients, x -dependent heat capacity, and reflectivity. Our results are interpreted in terms of relative phase composition of ejecta and discussed in application to experiments.

Josiah Bjorgaard
Los Alamos Natl Lab

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