

Abstract Submitted  
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**Effects of shear strain on initiation of chemical reactions in HMX**

ONISE SHARIA, MAIJA KUKLJA, The University of Maryland, College Park — We performed a theoretical study of detonation initiation reactions in crystalline  $\beta$ -HMX using ab-initio methods. A HONO formation and elimination and direct N-NO<sub>2</sub> bond dissociation are considered to be main mechanisms of detonation initiation in HMX. We calculated the activation barriers of these two reactions using nudged elastic band method. We studied the same reactions in HMX exposed to the shear strain in (001) and (101) directions. The shear strain has been modeled by constructing an interface between different layers of HMX. We observed a significant change in energy barriers with respect to bulk calculations. This indicates that the shear strain plays an important role in detonation initiation in HMX. The results obtained are consistent with previously observed trends in DADNE and TATB and may be used to reveal common features of high explosive initiation behaviors.

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