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**Large-Amplitude Deformation and Bond Breakage in Shock-Induced Reactions of Explosive Molecules** JEFFREY KAY, Sandia National Laboratories — The response of explosive molecules to large-amplitude mechanical deformation plays an important role in shock-induced reactions and the initiation of detonation in explosive materials. In this presentation, the response of a series of explosive molecules (nitromethane, 2,4,6-trinitrotoluene [TNT], and 2,4,6-triamino-1,3,5-trinitrobenzene [TATB]) to a variety of large-amplitude deformations are examined using ab initio quantum chemical calculations. Large-amplitude motions that result in bond breakage are described, and the insights these results provide into both previous experimental observations and previous theoretical predictions of shock-induced reactions are discussed.

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