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Theoretical Studies on the Reaction Pathways of Electronically Excited DAAF JASON QUENNEVILLE, Spectral Sciences, Inc., DAVID S. MOORE, Los Alamos National Laboratory — The use of temporally and spectrally shaped ultrafast laser pulses to initiate, as well as detect, high explosives is being explored at Los Alamos. High level ab initio calculations, presented here, are a vital support for this effort. The ground and excited electronic state potential energy surfaces of 3,3'-diamino-4,4'-azoxyfurazan (DAAF) have been investigated using multi-configurational SCF and electron correlation methods. We will describe the geometrical and energetic character of the excited state minima, reaction coordinates and conical intersections of DAAF. The mechanisms for both radiative and non-radiative quenching of excited state population as well as possible pathways for photochemical and spectroscopic control will be outlined.

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