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Exploring Reaction Mechanism on Generalized Force Modified Potential Energy Surfaces (G-FMPES) for Diels-Alder Reaction SANJIV JHA, Univ of Southern Mississippi, KATIE BROWN, Auburn University, GOPINATH SUBRAMANIAN, Univ of Southern Mississippi — We apply a recent formulation for searching minimum energy reaction path (MERP) and saddle point to atomic systems subjected to an external force. We demonstrate the effect of a loading modality resembling hydrostatic pressure on the trans to cis conformational change of 1,3-butadiene, and the simplest Diels-Alder reaction between ethylene and 1,3-butadiene. The calculated MERP and saddle points on the generalized force modified potential energy surface (G-FMPES) are compared with the corresponding quantities on an unmodified potential energy surface. Our study is performed using electronic structure calculations at the HF/6-31G** level as implemented in the AIMS-MOLPRO code. Our calculations suggest that the added compressive pressure lowers the energy of cis butadiene. The activation energy barrier for the concerted Diels-Alder reaction is found to decrease progressively with increasing compressive pressure.

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