Abstract Submitted
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Non-Adiabatic Molecular Dynamics of B+H2 DAVID WEEKS, LUKE BARGER, Air Force Institute of Technology — Adiabatic potential energy surfaces for the B+H2 system are used together with derivative coupling terms to compute diabatic potential energy surfaces. The diabatic surfaces are then expanded in terms of Legendre polynomials and represented in a mixed angular momentum, radial coordinate basis. This matrix representation of the potential is combined with the nuclear kinetic energy to yield a set of coupled differential equations that describe the non-adiabatic dynamics of B+H2. This dynamics is explored using numerical wave packet propagation.

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