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Title:	Beyond Born-Oppenheimer constructed diabatic potential energy surfaces for F + H ₂ reaction
Authors:	Shamasundar, K.R. (/jspui/browse?type=author&value=Shamasundar%2C+K.R.)
Keywords:	Potential Energy Surfaces Nonadiabatic Coupling Terms (NACTs) Born-Oppenheimer
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Abstract:	First principles based beyond Born-Oppenheimer theory has been implemented on the F + H ₂ system for constructing multistate global diabatic Potential Energy Surfaces (PESs) through the incorporation of Nonadiabatic Coupling Terms (NACTs) explicitly. The spin-orbit (SO) coupling effect on the collision process of the F + H ₂ reaction has been included as a perturbation to the non-relativistic electronic Hamiltonian. Adiabatic PESs and NACTs for the lowest three electronic states (12A', 22A', and 12A'') are determined in hyperspherical coordinates as functions of hyperangles for a grid of fixed values of the hyperradius. Jahn-Teller (JT) type conical intersections between the two A' states translate along C _{2v} and linear geometries in F + H ₂ . In addition, A' and A'' states undergo Renner-Teller (RT) interaction at collinear configurations of this system. Both JT and RT couplings are validated by integrating NACTs along properly chosen contours. Subsequently, we have solved adiabatic-to-diabatic transformation (ADT) equations to evaluate the ADT angles for constructing the diabatic potential matrix of F + H ₂ , including the SO coupling terms. The newly calculated diabatic PESs are found to be smooth, single-valued, continuous, and symmetric and can be invoked for performing accurate scattering calculations on the F + H ₂ system
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