Beyond Born-Oppenheimer Constructed Diabatic Potential Energy Surfaces for HeH$_2^+$

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First principles based beyond Born-Oppenheimer theory [1] has been employed to construct multi-state global Potential-Energy Surfaces (PESs) for the HeH$_2^+$ [2-7] system by explicitly incorporating the Nonadiabatic Coupling Terms (NACTs). Adiabatic PESs and NACTs for the lowest four electronic states ($1^2A'$, $2^2A'$, $3^2A'$ and $4^2A'$) are evaluated as functions of hyperangles for a grid of fixed values of the hyperradius in hyperspherical coordinates. [7] Conical intersection between different states are validated by integrating the NACTs along appropriately chosen contours. Subsequently, adiabatic-to-diabatic (ADT) [8] transformation angles are determined by solving the ADT equations to construct the diabatic potential matrix for the HeH$_2^+$ system [7] which are smooth, single-valued, continuous, and symmetric and are suitable for performing accurate scattering calculations for the titled system.

References: