Non-variational Density functional theory for predicting transition state geometries and barrier heights.

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Abstract:

For locating the first order saddle point geometries and calculating the barrier heights on a Born-Oppenhiemer potential energy surface, we have used Hartree-Fock orbital and non-local DFT employing Becke exchange and Lee-Yang-Parr correlation potential. By comparison to the available variational hybrid density functional and ab initio methods, we found that our non-variational DFT has an excellent cost-to performance ratio.