

# **Spin-Correct Spin-Flip Using ORMAS**

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The spin-flip method presents a powerful way to address complex problems, such as excited state potential energy surfaces, with the need to use time-consuming multi-configurational methods. A down side to spin-flip methods is that they are frequently subject to spin contamination that can vary significantly from region to region in a potential energy surface, thereby corrupting the associated energetics.

This presentation will demonstrate that the occupation restricted multiple active space (ORMAS) method can be used to provide spin-correct wave functions and therefore reliable energetics. The efficacy of the spin-flip ORMAS approach will be demonstrated for several applications.