

Linearized Coupled Cluster Corrections to Antisymmetrized Product of Strongly Orthogonal Geminals: role of dispersive interactions

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A linearized multi-reference Coupled Cluster (MR-LCC) theory is formulated based on the Antisymmetrized Product of Strongly Orthogonal Geminals (APSG) reference state. The role of dispersive interbond interactions is discussed. The presented theory has lead to qualitatively correct potential curves for the case when both OH bonds dissociate in H₂O, a result that cannot be achieved by adding only perturbative corrections to APSG. The potential curve obtained for the He...He problem practically coincides with the full CI (FCI) result, showing the unexpected accuracy of the MR-LCC approach in this case. We recently presented our results in the Journal of Chemical Theory and Computation [1].

[1] Zoboki, T., Szabados, Á., Surján, P. R. *J. Chem. Theory Comput.*, 9(6):2602-2608, **2013**.