Individually selecting MR-CI and MR Møller-Plesset Perturbation Theory: Method and Applications

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The DIESEL-CI (direct internal external separated individually selecting) program package has been extended by a Multi Reference Møller-Plesset Perturbation part. The selected wave function is used as perturbation reference while the perturbed wave function is expanded within the full MR-CI space. The resultant MP2/MP3-Energy may be used to perform the extrapolation to full MR-CI as an option to the traditionally employed Epstein-Nesbet based scheme. Several applications are presented in order to discuss improvements of accuracy in relation to computational cost.

Further there have been attempts to create a kind of "black box" CI with the aim to simplify the calculation of excited states and potential surfaces. The development is reported and illustrated on O_2 and CH+.