Examination of single- and multi-reference methods for the calculation of potential surfaces

Jeppe Olsen, Center for Theoretical Chemistry
Department of Chemistry, Aarhus

For a number of simple molecules, including HF, O_3, CU_2 and NO, potential surfaces are calculated using single- and multi-reference methods and compared where possible with full configuration interaction calculations. Of special interest is the comparison of pseudo-multi-reference coupled cluster methods using a commutative operator-manifold based upon a single reference-determinant with true multi-reference coupled cluster methods using non-commutative operator manifolds. It is shown that the true multi-reference methods and various approximations to these allows the most compact description of accurate wavefunctions.