Several single reference (SR-CC) coupled cluster methods are shown to work for traditionally multi-reference (MR) problems such as bond breaking subject to restricted Hartree-Fock (RHF) references. The correlated methods can successfully describe any MR problem with enough higher order clusters: singles and doubles (CCSD), singles, doubles and triples (CCSDT), singles, doubles, triples, and quadruples (CCSDTQ), etc. However, due to the steep increase in the computational cost, it is not practical to do larger systems or to use large basis sets without active space partitioning. In this study, the orbital space is partitioned into an active space subject to an unambiguous statistical criteria to span the MR behavior which defines an extended space to let the active space relax. The rest is considered the external space. The extended space is treated with CCSDT and the external space with CCSD. An automated scheme for determining the extended space is presented and evaluated. We build upon the tailored-CC scheme of Hino et al. and address its main shortcoming of neglecting the coupling between the active space and the rest of the orbital space which results in loss of accuracy as well as a pronounced nonparallelism error (NPE). The automated scheme makes it unnecessary for the user to judge whether a chosen active space is sufficient to correctly solve the problem.

We illustrate this method for the hydrogen fluoride and fluorine molecule ground state dissociation potentials using the extended space partitioning methods. Experimental accuracy for the dissociation energy is achieved at a small fraction of the cost of doing a full CCSDT calculation. This approach is easily amendable to higher order clusters which are required for double and triple bond breaking and other strongly multi-reference systems. The more challenging systems: ethylene twist and the isomerization of bicyclo[1.1.0]butane to trans -buta-1,3-diene are also presented.