Supplementary Material (ESI) for PCCP

Auxiliary material for:

Multireference perturbation theory can predict a false ground state

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The presented Auxiliary Materials reports the initial results obtained with NEVPT[1] for the $^3\Sigma_u^-$ and $^5\Sigma_u^-$ states of Sc2 employing the same basis set and complete active space used throughout the studies presented in this communication. Figure A shows the potential energy curves for the $^3\Sigma_u^-$ and $^5\Sigma_u^-$ states of scandium dimer, from which it is clear that in the absence of intruder states the ground state of scandium dimer is $^5\Sigma_u^-$.

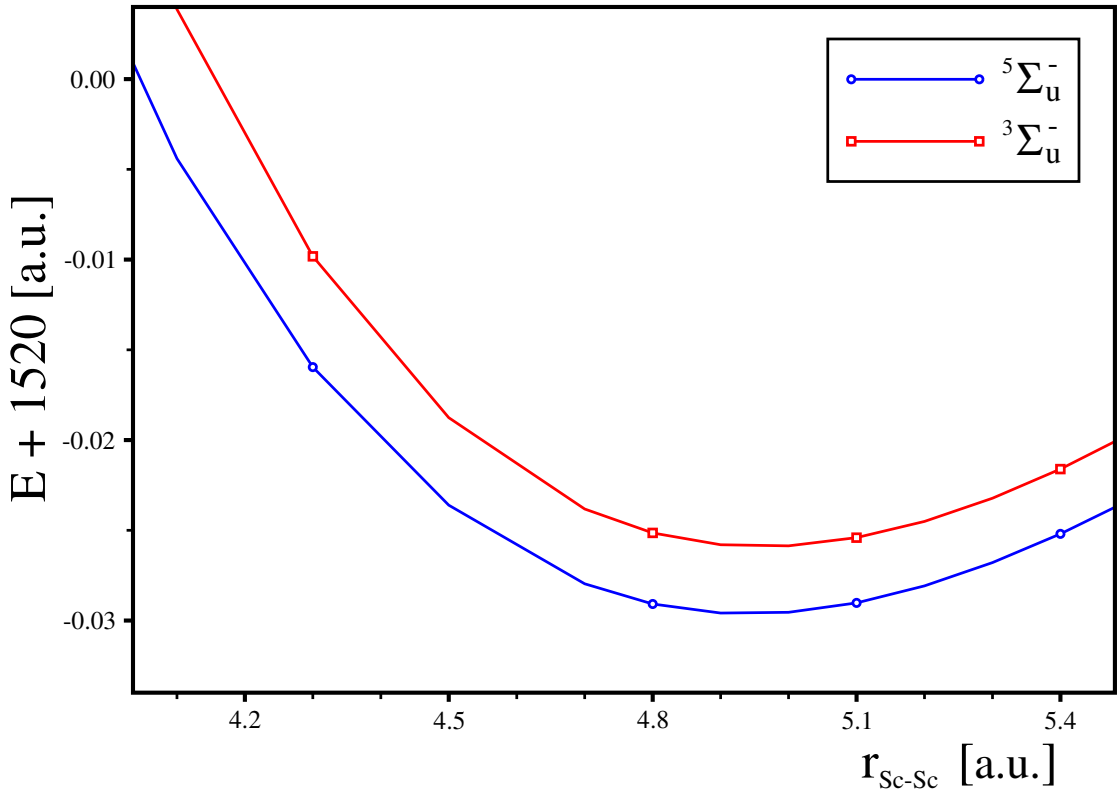

FIG. A. Potential energy curves for the $^5\Sigma_u^-$ and $^3\Sigma_u^-$ states obtained with the NEVPT2 method.

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[1] C. Angeli, R. Cimiraglia, S. Evangelisti, T. Leininger and J.-P. Malrieu, *J. Chem. Phys.*, 2001, **114**, 10252.