Multiconfigurational treatments of positron containing complexes

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In this work, multi-component calculations of the interaction of positrons with atoms, molecular, and molecular clusters are carried out. Positrons can serve as a probe to the electronic structure of a physical system, however the study of these types of systems requires a systematically improvable treatment of the interaction of positrons with atoms, molecular, and molecular clusters. The approach taken in this work involves both mean-field and post mean-field treatments of multi-component systems. Bound positrons occupy a diffuse orbital, and the positron affinities are sensitive to the treatment of electron-electron and electron-positron correlations. Nonvalence correlation bound (NVCB) anions display a similar behavior with the excess electron occupying diffuse orbitals and the electron affinity being sensitive to the treatment of electron correlation. Motivated by our previous work on NVCB anions, we demonstrate a method to construct compact, tailored configuration interaction wave functions for these systems. Additionally, these multiconfigurational wave functions are used for subsequent fixed-node diffusion Monte Carlo (DMC) calculations and compared to DMC calculations with mean field trial wave functions.