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Quantitative characterization of the errors of the 3d-transition-metal pseudopotentials in Diffusion Monte Carlo ALLISON DZUBAK, JARON KROGEL, FERNANDO REBOREDO, Oak Ridge National Laboratory — Using a recently proposed extrapolation scheme and multideterminent wavefunctions, we estimate the errors of two families of non-local pseudopotentials of the first row transition metal atoms Sc-Zn. Jastrow sensitivities are presented to assess the quality of two sets of pseudopotentials with respect to localization error reduction. The locality approximation and T-moves scheme are also compared for accuracy of total energies. After removal of the locality and T-moves errors, we present the range of fixed-node energies between a single determinant description and a full valence multideterminant CAS expansion. The results presented here corroborate previous findings that the locality approximation is less sensitive to changes in the Jastrow than T-moves, yielding more accurate total energies. For both the locality approximation and T-moves, we find decreasing Jastrow sensitivity moving left to right across the series Sc-Zn. The recently generated pseudopotentials of Krogel et al. reduce the magnitude of the localization error compared with the pseudopotentials of Burkatzki et al. For the Sc-Zn atomic series with these pseudopotentials, and using up to three-body Jastrows we find that the fixed-node error is dominant over the localization error.

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