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Testing of He-core pseudopotentials for 3d elements in quantum Monte Carlo MINYI ZHU, LUBOS MITAS, North Carolina State University — We construct He-core pseudopotentials for several elements in the 3rd row such as for V, Cr, Mn, Fe and Zn, with the goal of using these in high-accuracy quantum Monte Carlo (QMC) calculations. We study the accuracy of constructed pseudopotentials on MnO molecular states with different spin polarizations. We compare these results also with Density Functional Theory and Hartree-Fock approaches since we previously found noticeable differences between Ne-core pseudopotential and relativistic all-electron calculations in high-spin vs. low-spin state comparisons. The result indicates that these discrepancies stem from method biases related to the presence of core states, as we conjectured earlier. Additionally, we also discuss the computational cost of the He-core pseudopotentials in QMC calculations.

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