Nearly-exact calculation of chromium dimer binding with auxiliary-field quantum Monte Carlo\textsuperscript{1} WIRAWAN PURWANTO, SHIWEI ZHANG, HENRY KRAKAUER, College of William and Mary — The binding of the strongly correlated $\text{Cr}_2$ molecule has long resisted accurate theoretical description, and $\text{Cr}_2$ has become a landmark test for many-body computational methods. We first performed exact auxiliary-field quantum Monte Carlo (AFQMC) calculations using a moderately-sized basis set. In parallel, phaseless AFQMC\textsuperscript{2} calculations were carried out using the same and larger basis sets to remove the finite-basis errors from the exact AFQMC calculations. Results on $\text{Cr}_2$ ground-state properties, including binding energy, equilibrium distance, and vibrational frequency, are in excellent agreement with experiment.

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