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Nearly-exact calculation of chromium dimer binding with auxiliary-field quantum Monte Carlo[1] WIRAWAN PURWANTO, SHIWEI ZHANG, HENRY KRAKAUER, College of William and Mary — The binding of the strongly correlated Cr_2 molecule has long resisted accurate theoretical description, and 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[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 Cr_2 ground-state properties, including binding energy, equilibrium distance, and vibrational frequency, are in excellent agreement with experiment.

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[2]Zhang and Krakauer, *Phys. Rev. Lett.* **90**, 136401 (2003)

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