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Possible calcium centers for hydrogen storage applications: An accurate many-body study by AFQMC calculations with large basis sets[1]
WIRAWAN PURWANTO, HENRY KRAKAUER, SHIWEI ZHANG, YUDISTIRA VIRGUS, College of William and Mary — Weak H_2 physisorption energies present a significant challenge to first-principle theoretical modeling and prediction of materials for H storage. There has been controversy regarding the accuracy of DFT on systems involving Ca cations. We use the auxiliary-field quantum Monte Carlo (AFQMC) method[2] to accurately predict the binding energy of Ca^+ - $4H_2$. AFQMC scales as N^3_{basis} and has demonstrated accuracy similar to or better than the gold-standard coupled cluster CCSD(T) method. We apply a modified Cholesky decomposition to achieve efficient Hubbard-Stratonovich transformation in AFQMC at large basis sizes. We employ the largest correlation consistent basis sets available, up to Ca/cc-pCV5Z, to extrapolate to the complete basis limit. The calculated potential energy curve exhibits binding with a double-well structure.

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[2]S. Zhang and H. Krakauer, Phys. Rev. Lett. **90**, 136401 (2003); W. A. Al-Saidi, S. Zhang and H. Krakauer, J. Chem. Phys. **124**, 224101 (2006).

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