Abstract Submitted
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Potential Energy Curves and Excited States of the C_2 Molecule by Auxiliary-Field Quantum Monte Carlo (AFQMC)[1] WIRAWAN PURWANTO, HENRY KRAKAUER, SHIWEI ZHANG, College of William and Mary, WISSAM AL-SAIDI, Cornell University — The accurate determination of potential energy curves (PECs) and excited states represents two difficult problems in electronic structure calculations. We present AFQMC PECs of the challenging C_2 molecule, focusing on the ground state and two singlet low-lying excited states. AFQMC calculates a target many-body wave function (WF) by means of random walks in the space of Slater determinants. We employ truncated complete active space (CAS) trial WFs (Ψ_T) to guide the AFQMC projection to obtain the desired state. With the phase-free constraint,[2] the CAS Ψ_T is effective in controlling the sign/phase problem, and filtering in the desired excited state. The AFQMC results are in very good agreement with exact results. Comparison with experimental spectroscopic constants will also be presented.

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

Wirawan Purwanto
College of William and Mary

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