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Quantum Monte Carlo Studies of Zinc-Porphyrin and Molybdenum dimer ADEM HALIL KULAHLIOGLU, LUBOS MITAS, North Carolina State University, Physics Department — We present fixed-node diffusion Monte Carlo (FN-DMC) studies focused on the calculation of vertical excitation energy in Q band corresponding to the excitation between the singlet ground-state (1^1A_g) and the lowest-lying singlet excited state (1^1E_u) of Zinc-Porphyrin (ZnP) molecule and the binding energy of the ground-state Molybdenum dimer (Mo_2). In the ZnP study, several trial wave functions for the excited state such as CIS, TDDFT and others were tested. We have obtained a very good agreement both with experiments and with high accuracy basis set correlated wave function calculations. The calculations show that the studied excitation is not well described by single-reference trial wave functions. In the Mo_2 study, the bias introduced by the fixed-node approximation with single-reference trial function is significant so we attempt to reduce it by means of the selected Configuration Interaction (selected-CI) technique. The single-particle orbitals that appear to lead to the lowest fixed-node error were generated by the hybrid version of the TPSS meta-GGA (TPSSh) functional. In this way, we have obtained significant improvements over the results from the single-reference trial function.

Adem Halil Kulahlioglu
North Carolina State University, Physics Department

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