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**Development of multicomponent semistochastic quantum Monte Carlo method for variational solution of molecular Hamiltonian without invoking the Born-Oppenheimer approximation** BENJAMIN ELLIS, ARINDAM CHAKRABORTY, Dept. of Chemistry, Syracuse University, ADAM HOLMES, HITESH CHANGLANI, CYRUS UMRIGAR, Dept. of Physics, Cornell University — We present the multicomponent extension of the semistochastic quantum Monte Carlo (mc-SQMC) method for treating electron-nuclear correlation in the molecular Hamiltonian. All particles in the molecule are treated quantum mechanically and the variational solution is obtained with the SQMC method. The key feature of this approach is that the BO and separation-rotor approximation are not assumed. The application of the SQMC method for multicomponent systems involves many formidable challenges and this talk will focus on strategies to address these challenges including, appropriate coordinate system for the molecular Hamiltonian, separation of the center of mass kinetic energy, construction of the 1-particle basis functions for electrons and nuclei, construction of the multicomponent CI space and evaluation of connected configurations needed during propagation step in the SQMC method. Results from mc-SQMC will be presented for $H_2$, $He_2$, and $H_2O$ systems. The $H_2$ system has been extensively studied using various methods, such as QMC and PIMC, making it an ideal system to test and compare the mc-SQMC implementation. The impact of the BO approximation and vibration-rotation coupling will be discussed by comparing mc-SQMC results with reported values for the weakly bound $He_2$.

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