# Accurate Determination and Prediction of Dipole-Bound States Using QMC

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Molecules with a dipole moment greater than 1.625D may form dipole-bound anions whose extra electron is diffusively distributed and far away from the positive center of the dipole (10-100Å). The theoretical description of weakly-bound anions remains a challenge, due in part to the relative weakness of the dipole interaction. Coupled cluster (CC) methods are known to be the only methods that can correctly obtain dipole-bound electron affinities so far. Nevertheless, CC methods are limited by their computational demand (they scale as $N^6$ or higher ). Quantum Monte Carlo (QMC) methods are a promising alternative to conventional wave function techniques when high accuracy is required with favorable $N^3$ scaling. In this work, correlated sampling-based phaseless Auxiliary-Field QMC (ph-AFQMC) and Variational Monte Carlo (VMC) optimization followed by Diffusion Monte Carlo (DMC) simulations were shown to accurately obtain the electron affinities for various dipole-bound anions with dipole moments that are slightly larger than the theoretical threshold.