Applying fully quantum embedded full configuration interaction quantum Monte Carlo to bond dissociation

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We present proof of concept results for the fully quantum embedded full configuration interaction quantum Monte method. In this fully quantum method, we embed the intiator version of full configuration interaction in density functional theory, called i-FCIQMC-in-DFT. Here we show that that i-FCIQMC-in-DFT has comparable accuracy to coupled cluster singles and doubles with perturbative triples embedded in density functional theory, CCSD(T)-in-DFT, by calculating dissociation energies of diatomic systems physisorbed on benzene. In addition, by generating a dissociation curve of hydrogen fluoride on benzene we show improvement over CCSD(T)-in-DFT in the bond breaking region.