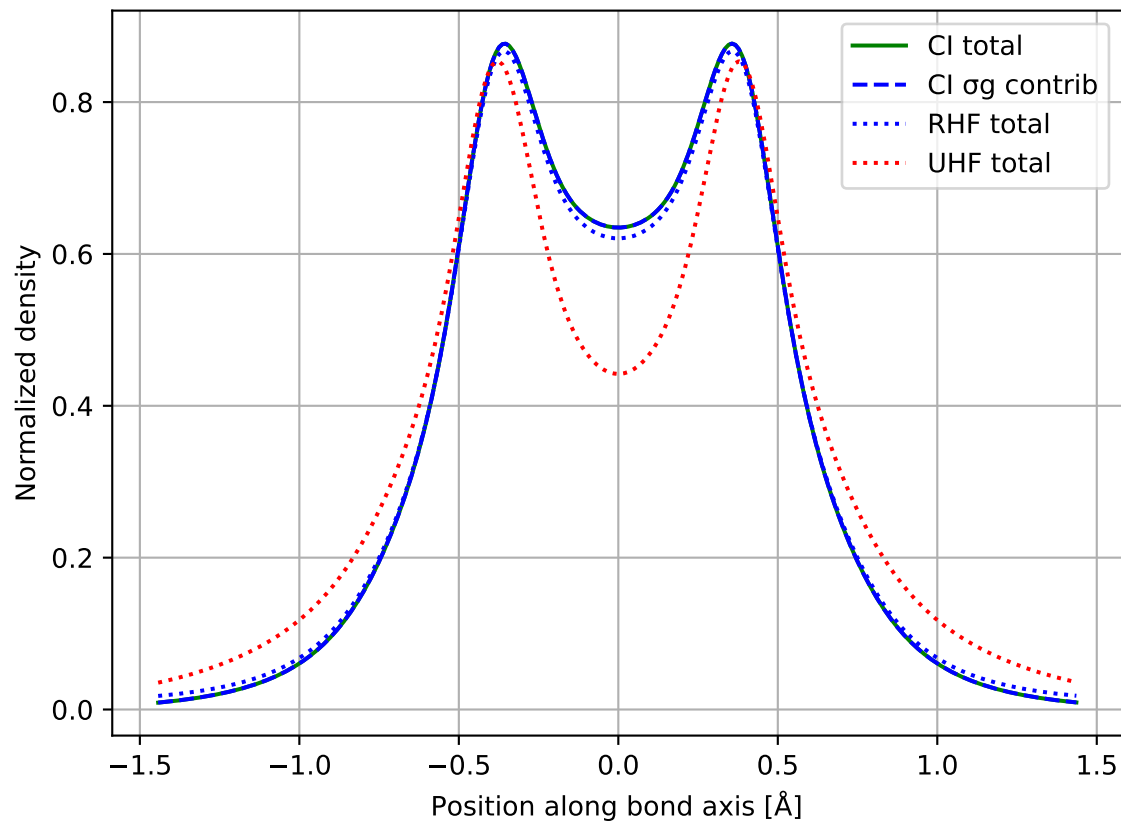


Equilibrium (CI from RHF orbitals)  
R=1.45 bohr



Max Separation (CI from UHF orbitals)  
R=8.00 bohr

