Multi-component molecular methods for hydrogen bonded systems and positronic compounds

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Recently, we have developed some first-principles approaches for multi-component systems including both electrons and nuclei (or positron) quantum-mechanically: (I) Multi-component molecular orbital (MC_MO) [1, 2], DFT (MC_DFT) [3], quantum Monte Carlo (MC_QMC) [4], and (II) *ab initio* path integral (PI) [5, 6] methods.

First, we demonstrated that HCN, as the simplest nitrile molecule, can bind a positron by the most accurate QMC approach [4]. We have also found that the positron affinity (PA) value of acetonitrile with electronic 6-31++G(2df,2pd) and positronic [15s15p3d2f1g] basis set with the CI scheme of MC_MO method is calculated as 4.96 mhartree [2], which agrees to within 25% with the recent experimental value of 6.6 mhartree by Danielson *et al*. [7].

Next, we will show some theoretical aspects of path integral simulation with 2nd and 4th order Trotter expansion. Then, we will show some computational results with PIMD simulation for the H/D isotope effect on deprotonated water dimer anion $H_3O_2^-$ [5,6] and muonated molecular systems.

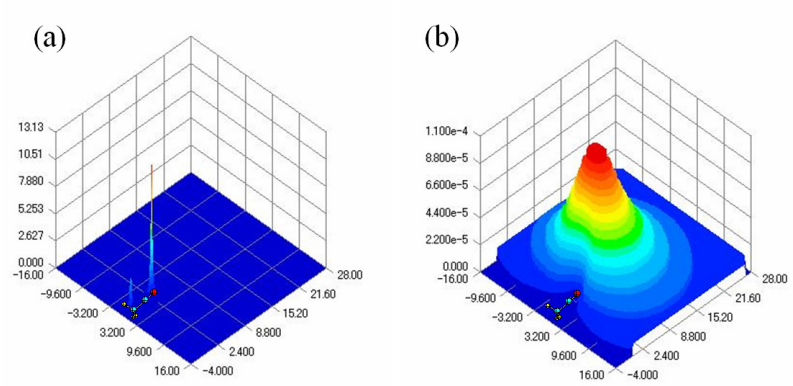

Figure 1: (a) Electronic and (b) positronic densities of [CH_3CN; e^+] species.

References

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