A Verification to One of Limitations of DFT

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In the article written by Yang Weitao (DOI: 10.1126/science.1158722), there are several spectacular errors that can be characterized and understood through binding curves, the perspective of fractional charges and fractional spins.

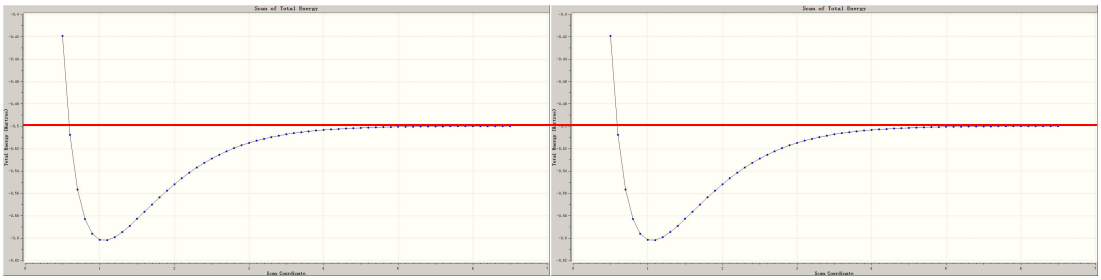
As shown in the paper, the binding curves of H_2^+ computed by B3LYP and LDA are compared with the curve by HF. For verifying other DFT methods, some of them have been applied.

The methods have been used are shown below:
1, HF and CCSD (as the Golden standard)
2, PBE and BLYP
3, B3LYP, M06-2X, and ωB97XD
4, B2PLYP

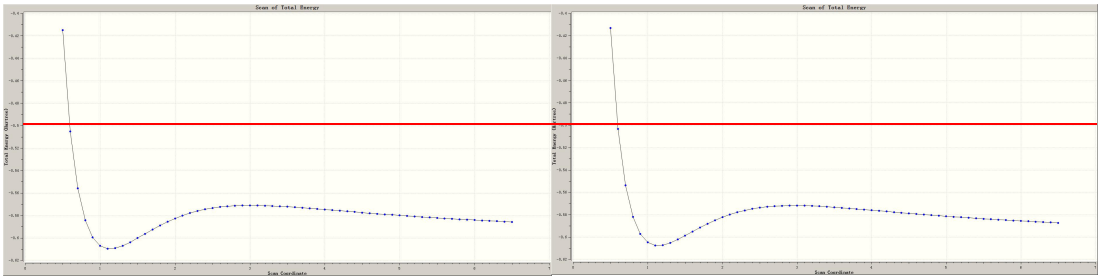
As the mission of scan in Gaussian 09, the distance of two H atoms is scanned from 0.5 Å to 6.5 Å, and completed in 60 steps.

In these works, aug-cc-pVTZ is worked as basis set. All of computations is done via Gaussian 09 D.01 program package.

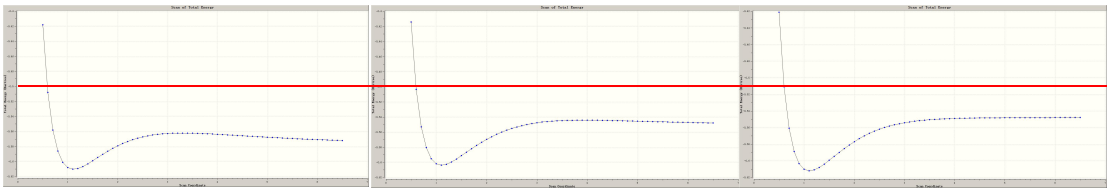
The binding curves of H_2^+ are plotted below:
1, HF(left) and CCSD(right)



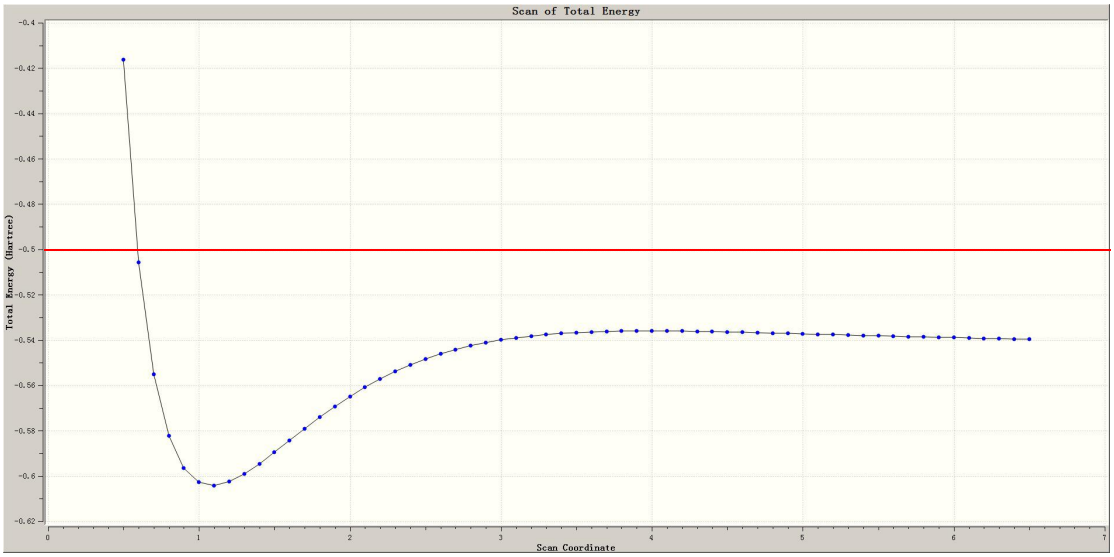
2, PBE(left) and BLYP(right)



3, B3LYP(left), M06-2X(middle), and ωB97XD(right)



4, B2PLYP



Honestly, it is true that all of DFT methods in my paper fail to describe the binding curve of H_2^+, although the tend of curves is in keeping with the ones of standard methods.