Supporting Information to "Electric Field induced Activation of H_2 - Can DFT do the Job?"†

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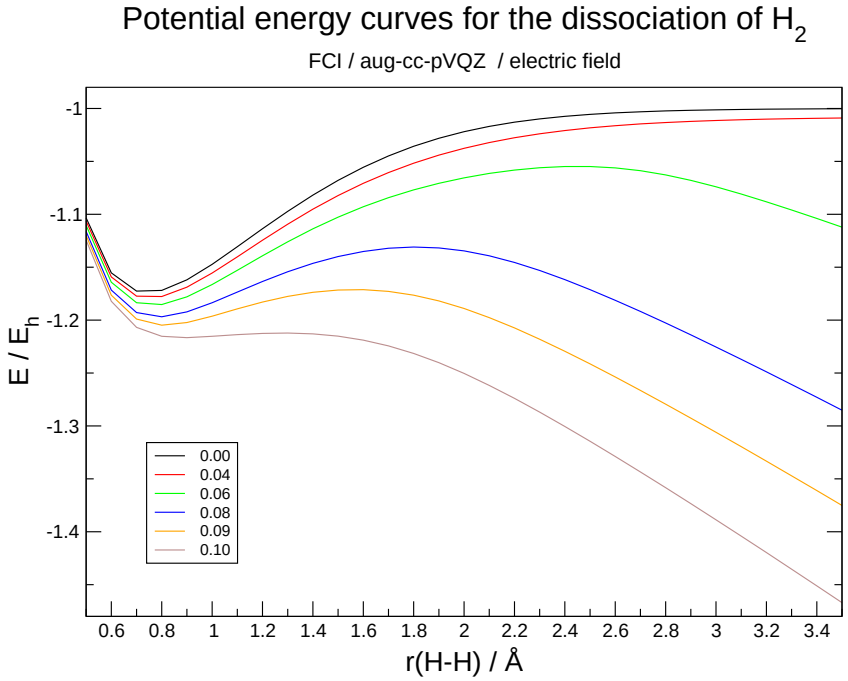
This Supporting Information contains the remaining data mentioned but not discussed in the main article. All the data is presented in the form of graphs showing the energy vs. the H-H-distance.

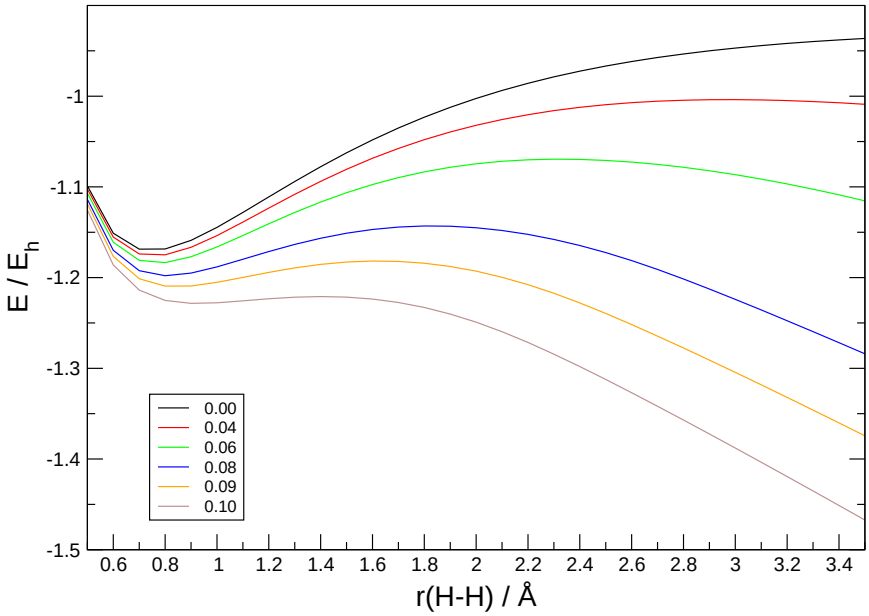
In the first part of this ESI one group of plots is given. Here different colours represent different strengths of the electric field the value of which is given in the legend (field strength in atomic units - 1. a.u. = 5.4122 * 10^{11} Vm^{-1}; for further information on the methods used see main article).

In the second part of the ESI all four graphs for one field strength are plotted together to simplify comparison between the different methods.



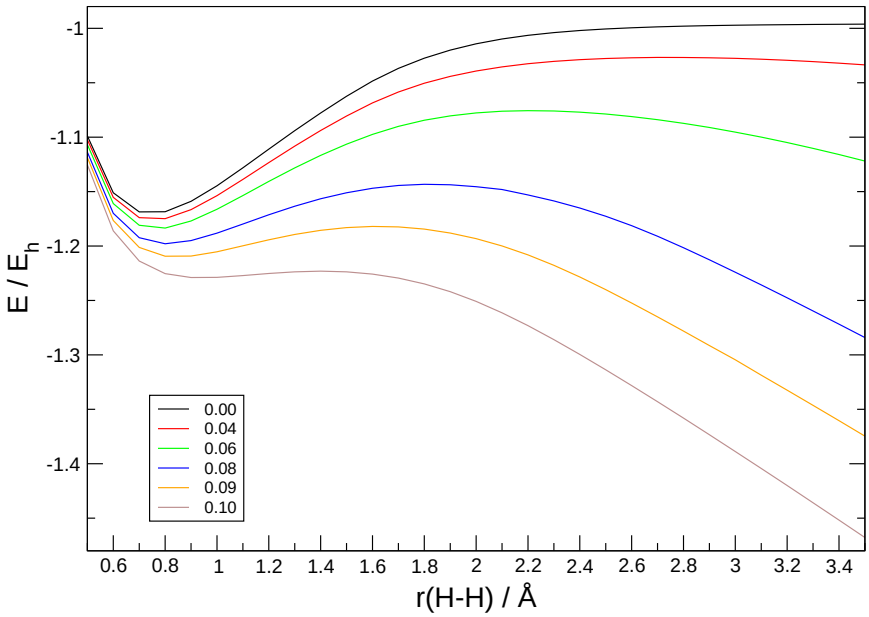
Potential energy curves for the dissociation of H_2

R-BLYP / aug-cc-pVQZ / electric field



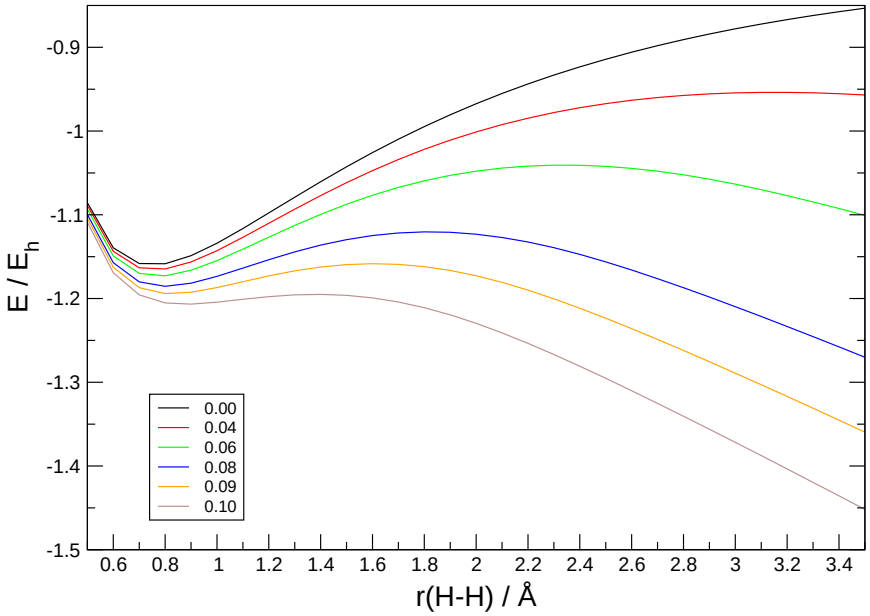
Potential energy curves for the dissociation of H_2

U-BLYP / aug-cc-pVQZ / electric field



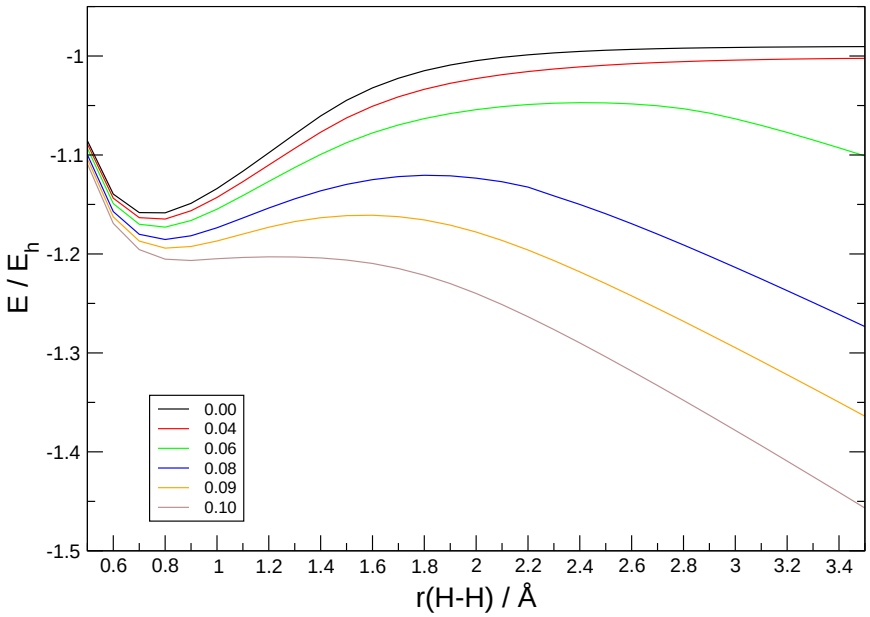
Potential energy curves for the dissociation of H_2

R-LC-BLYP / aug-cc-pVQZ / electric field



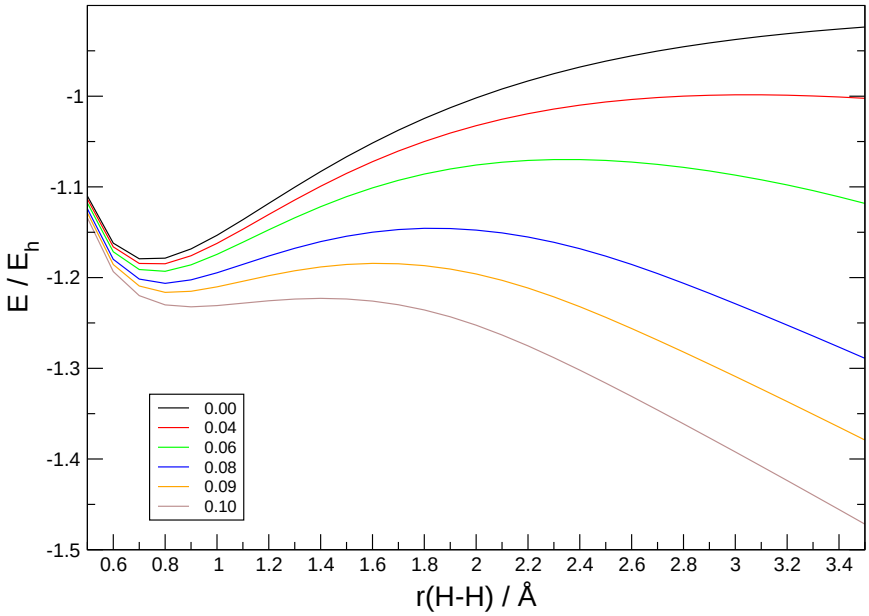
Potential energy curves for the dissociation of H_2

U-LC-BLYP / aug-cc-pVQZ / electric field



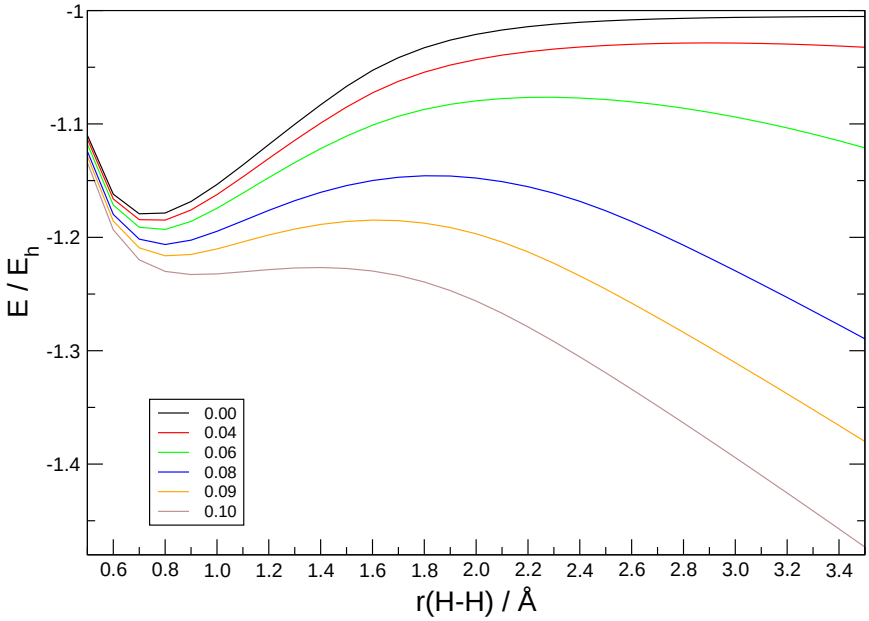
Potential energy curves for the dissociation of H_2

R-B3LYP / aug-cc-pVQZ / electric field



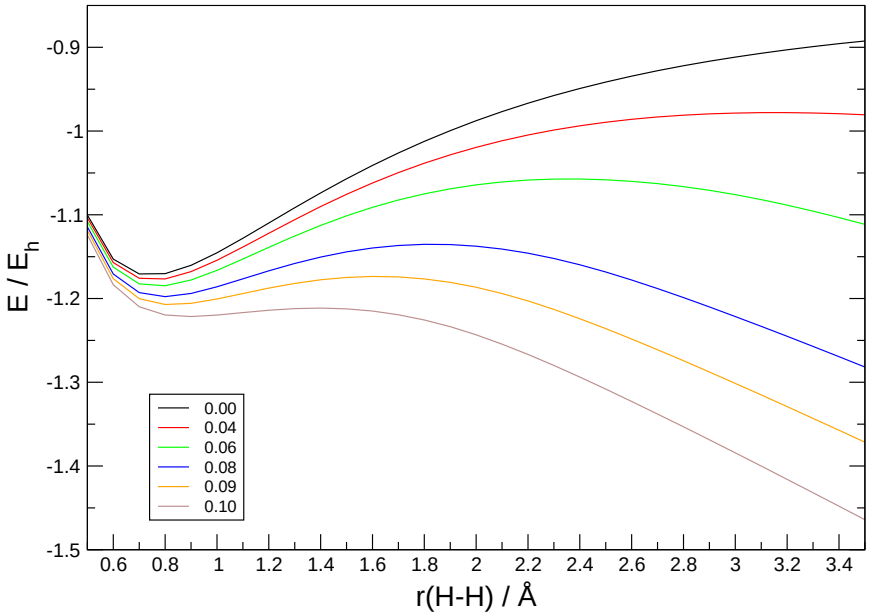
Potential energy curves for the dissociation of H_2

U-B3LYP / aug-cc-pVQZ / electric field



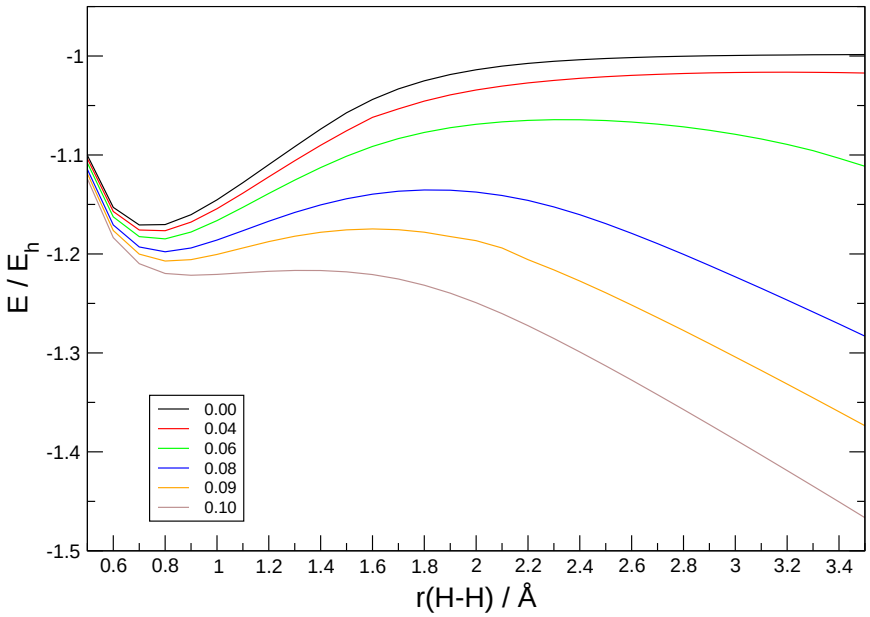
Potential energy curves for the dissociation of H_2

R-CAM-B3LYP / aug-cc-pVQZ / electric field



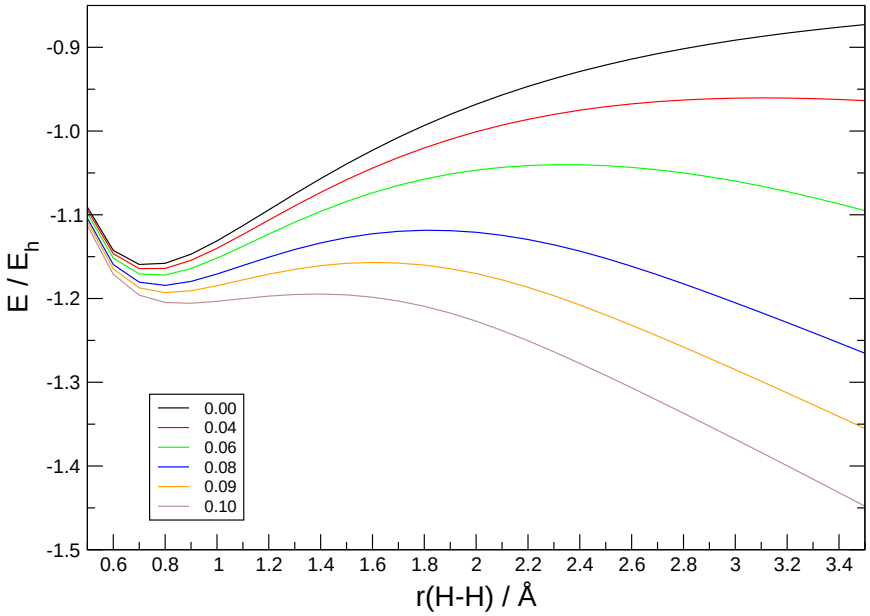
Potential energy curves for the dissociation of H_2

U-CAM-B3LYP / aug-cc-pVQZ / electric field



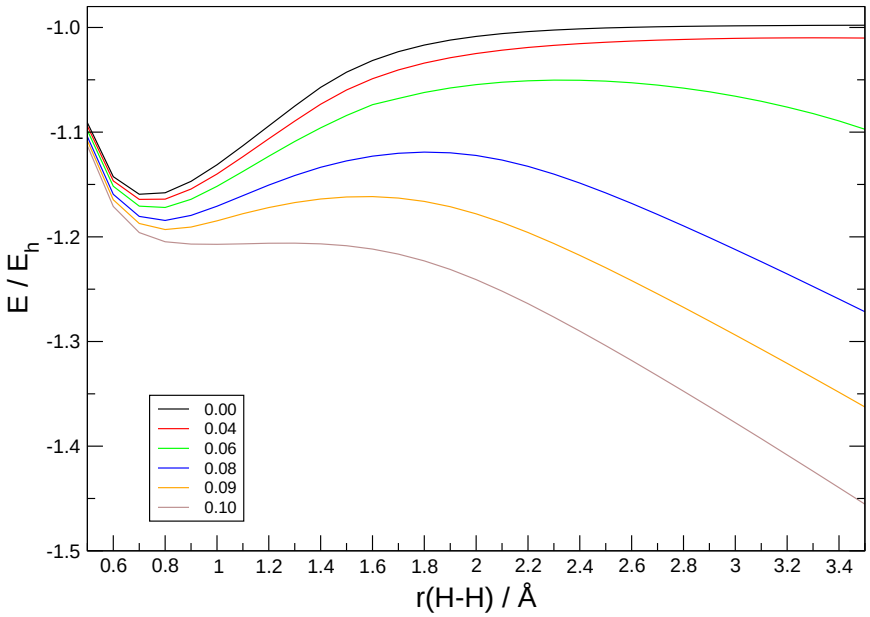
Potential energy curve for the dissociation of H_2

R-B2LYP / aug-cc-pVQZ / electric field



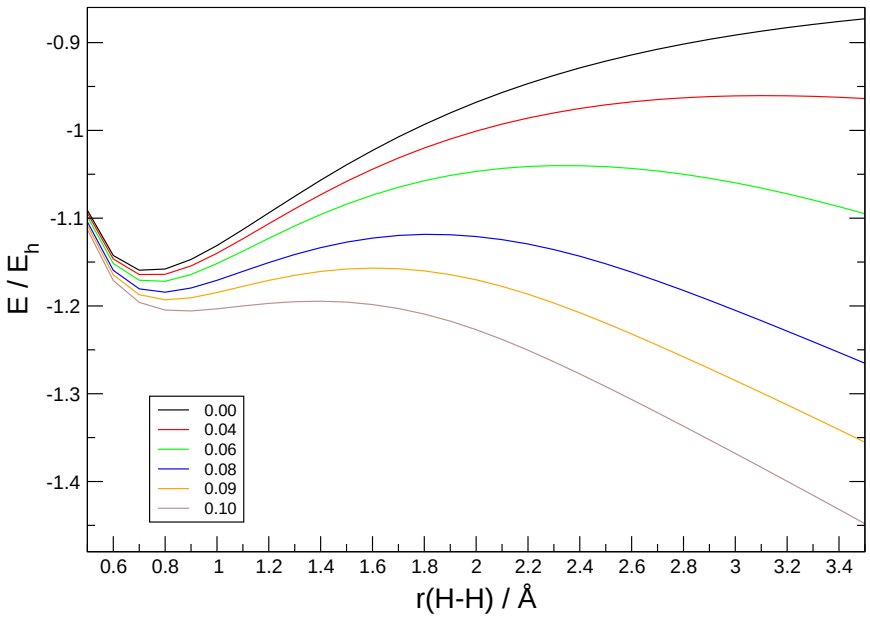
Potential energy curve for the dissociation of H_2

U-B2LYP / aug-cc-pVQZ / electric field



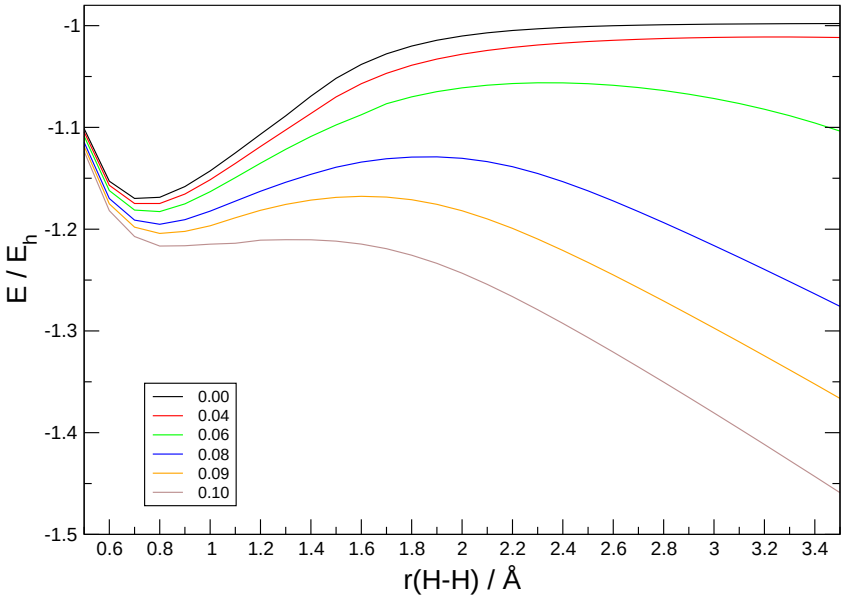
Potential energy curves for the dissociation of H_2

R-B2PLYP / aug-cc-pVQZ / electric field



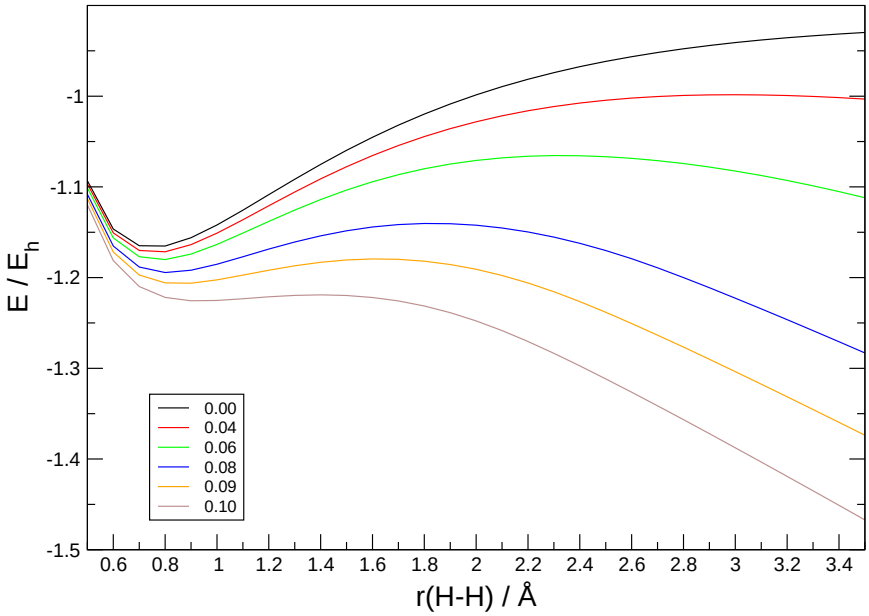
Potential energy curve for the dissociation of H_2

U-B2PLYP / aug-cc-pVQZ / electric field



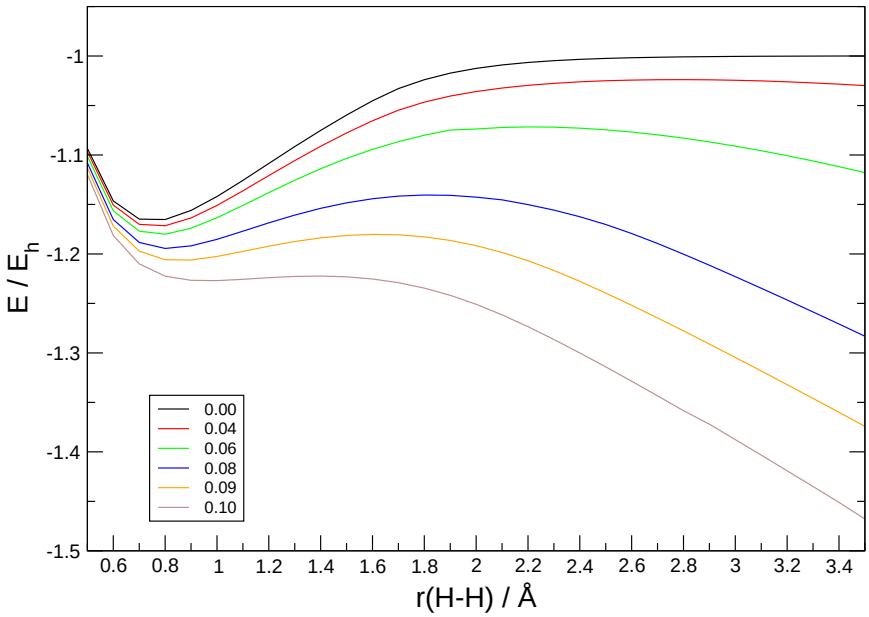
Potential energy curves for the dissociation of H_2

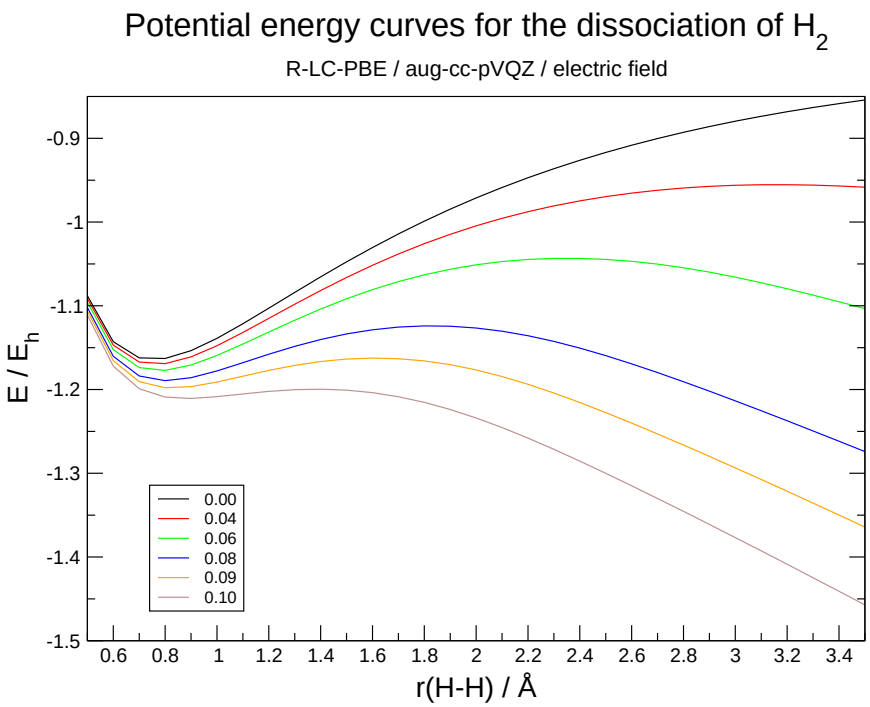
R-PBE / aug-cc-pVQZ / electric field

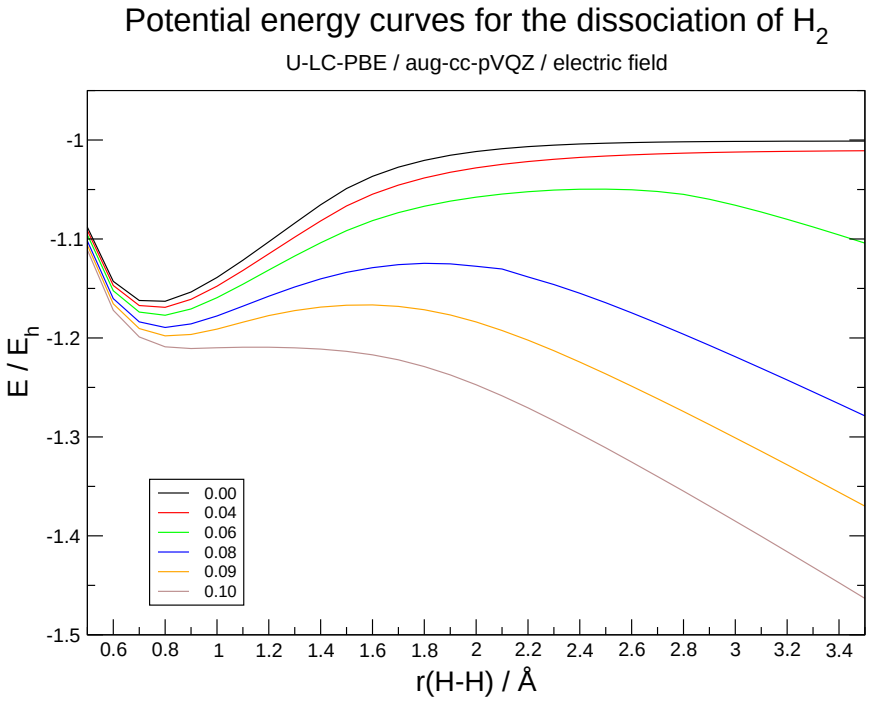


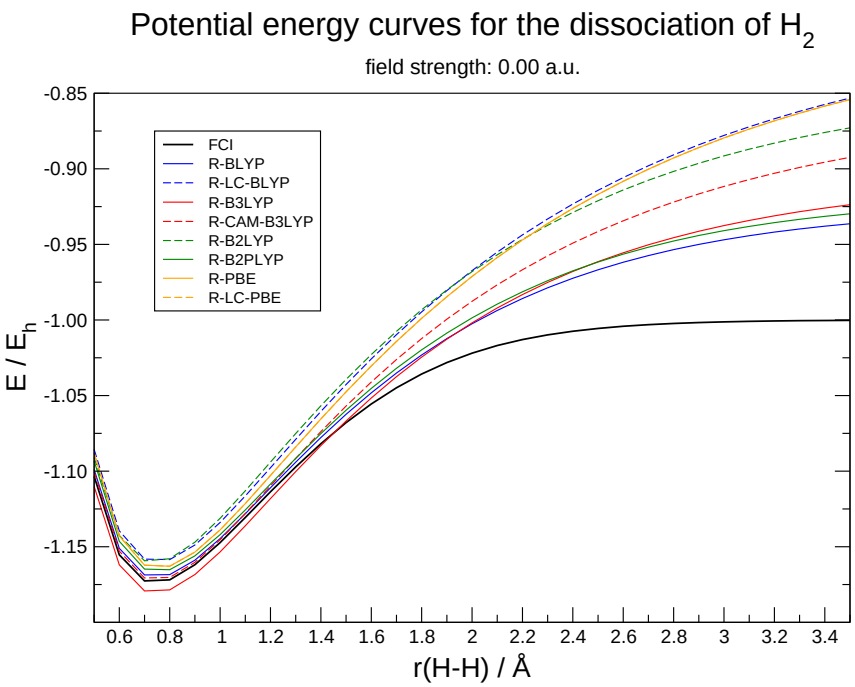
Potential energy curves for the dissociation of H_2

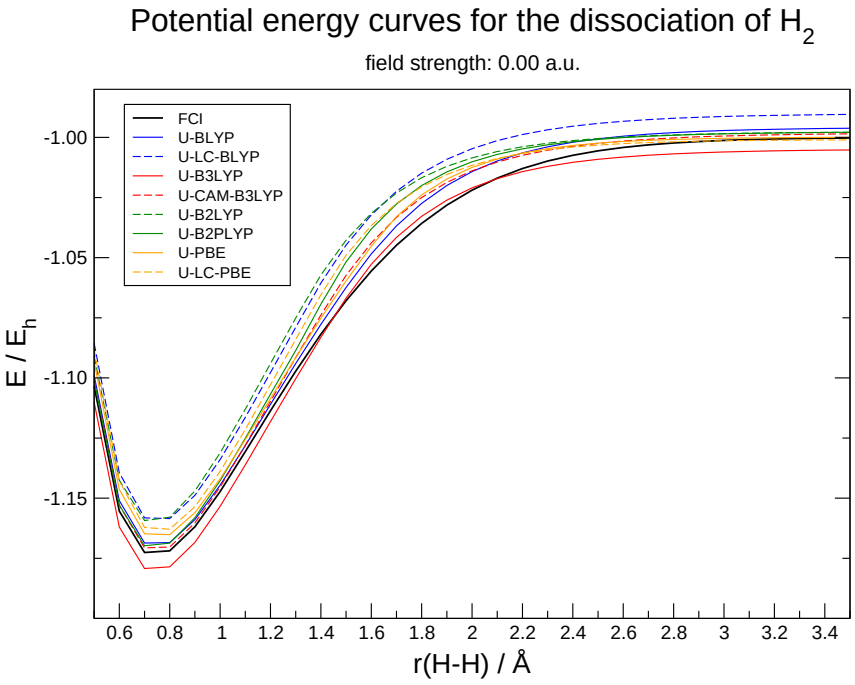
U-PBE / aug-cc-pVQZ / electric field

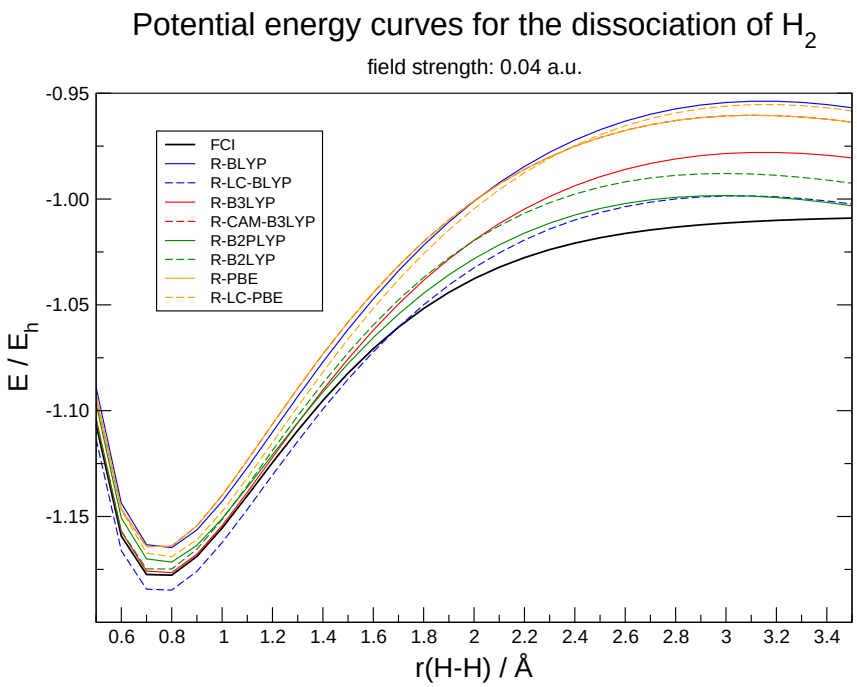


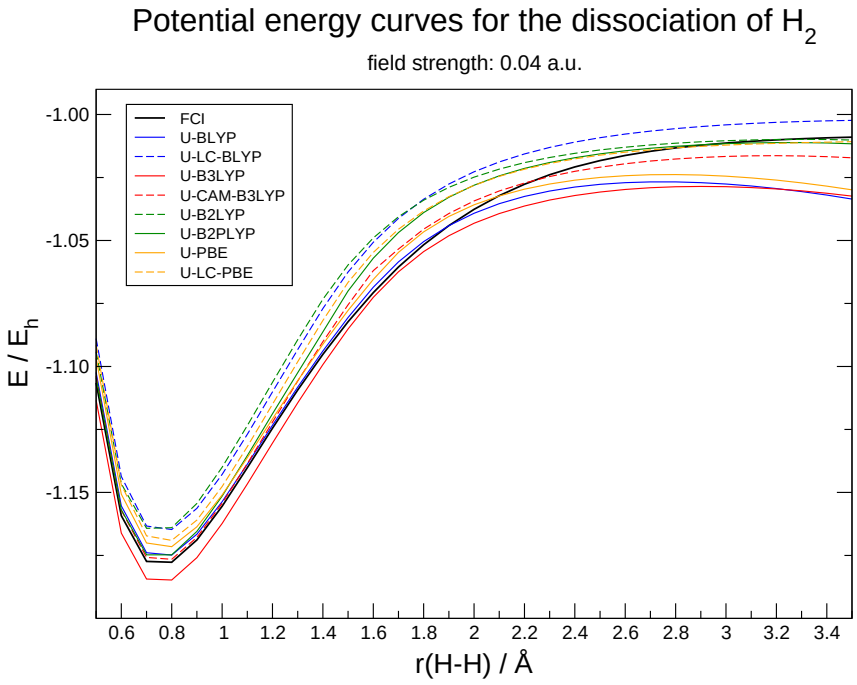


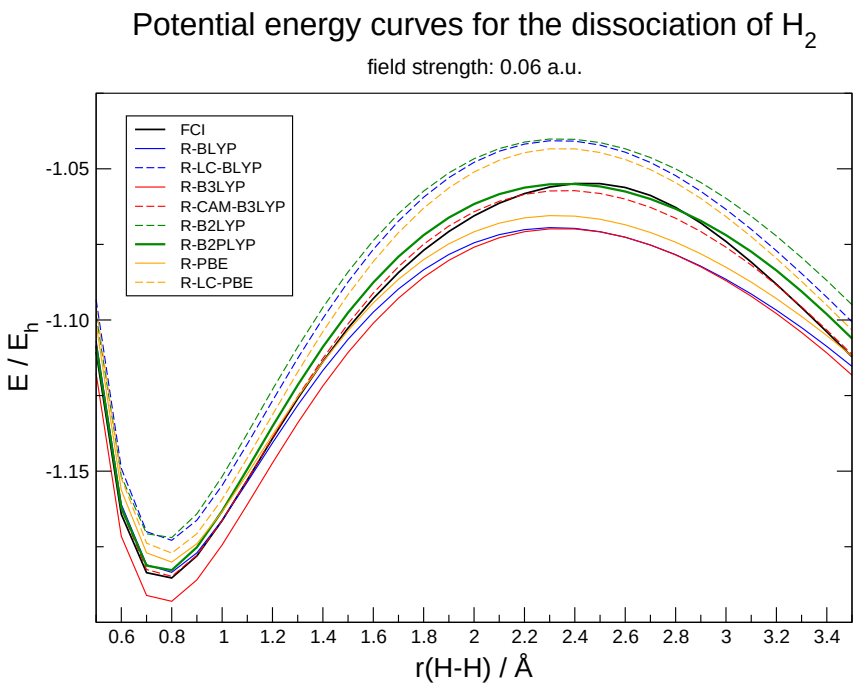


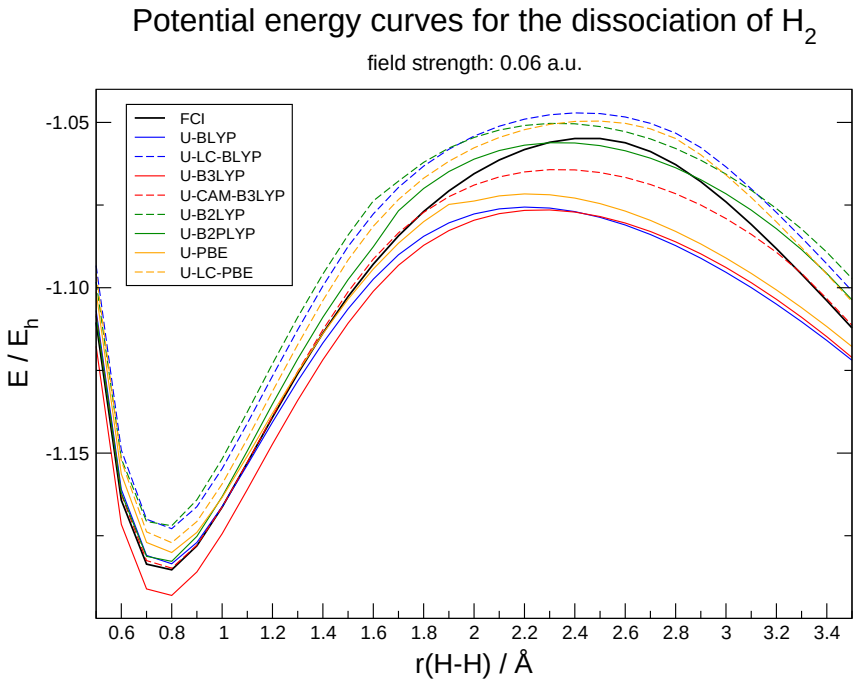

Potential energy curves for the dissociation of H2
field strength: 0.00 a.u.
FCI
R-BLYP
R-LC-BLYP
R-B3LYP
R-CAM-B3LYP
R-B2LYP
R-B2PLYP
R-PBE
R-LC-PBE
E / Eh
r(H-H) / Å

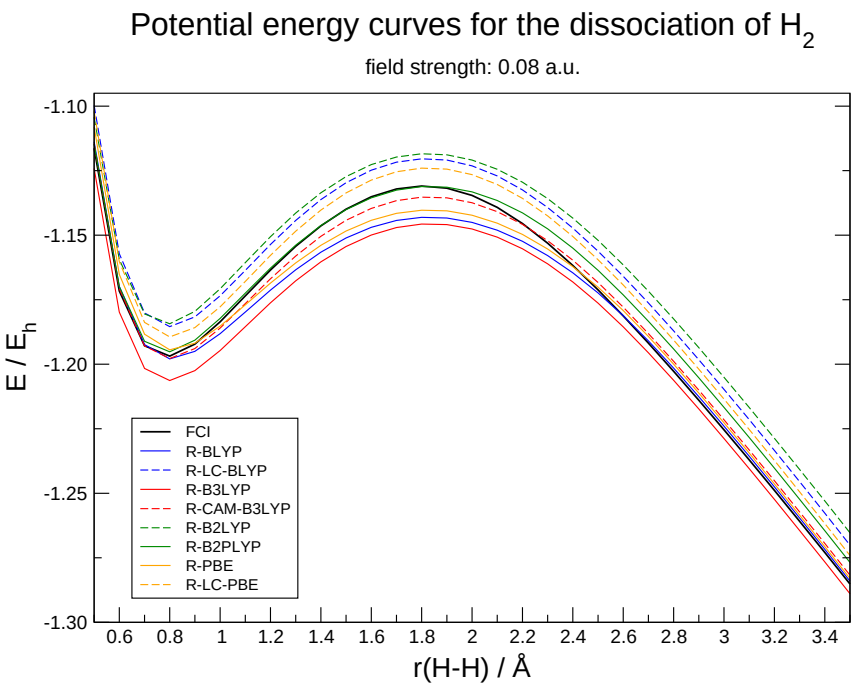

Potential energy curves for the dissociation of H2
field strength: 0.00 a.u.
FCI
U-BLYP
U-LC-BLYP
U-B3LYP
U-CAM-B3LYP
U-B2LYP
U-B2PLYP
U-PBE
U-LC-PBE
E / Eh
r(H-H) / Å

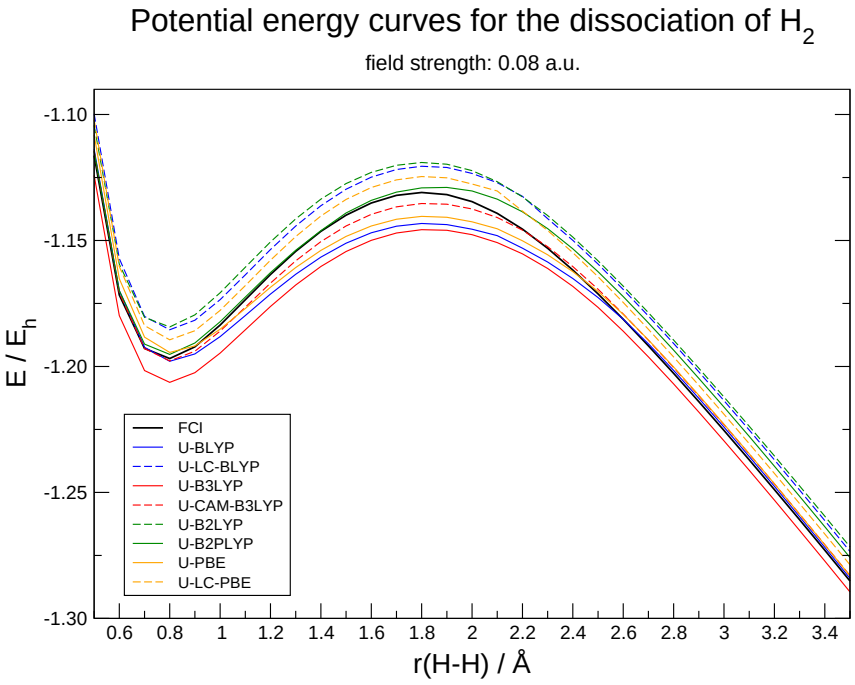


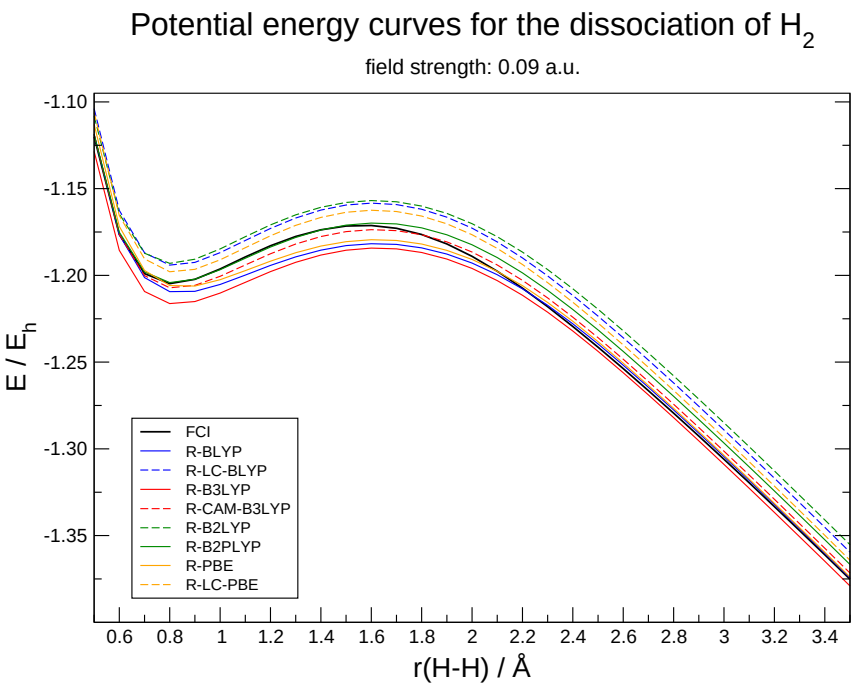


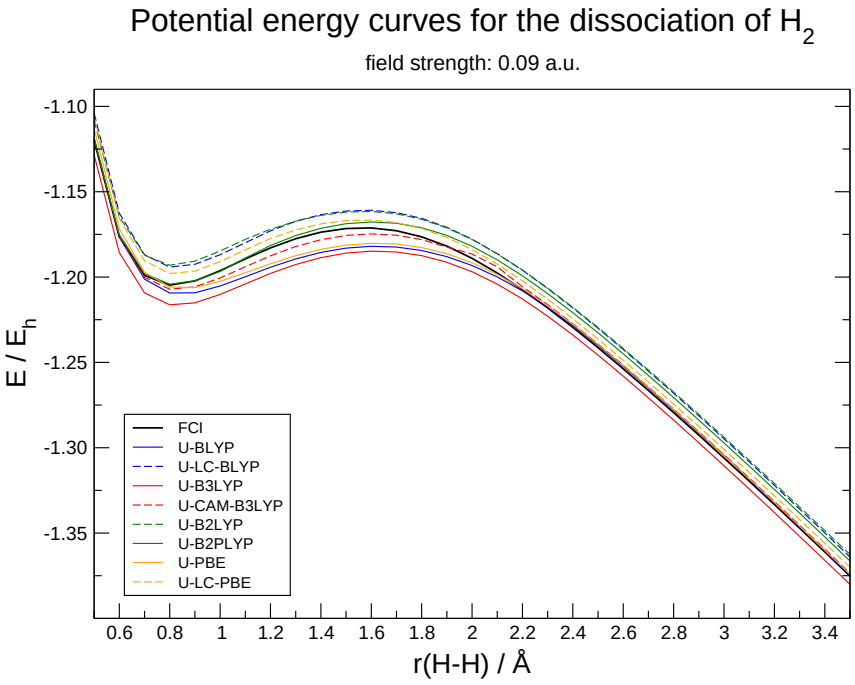

Potential energy curves for the dissociation of H2
field strength: 0.06 a.u.
FCI
R-BLYP
R-LC-BLYP
R-B3LYP
R-CAM-B3LYP
R-B2LYP
R-B2PLYP
R-PBE
R-LC-PBE
E / Eh
-1.05
-1.10
-1.15
0.6
0.8
1
1.2
1.4
1.6
1.8
2
2.2
2.4
2.6
2.8
3
3.2
3.4
r(H-H) / Å


Potential energy curves for the dissociation of H2
field strength: 0.06 a.u.
FCI
U-BLYP
U-LC-BLYP
U-B3LYP
U-CAM-B3LYP
U-B2LYP
U-B2PLYP
U-PBE
U-LC-PBE
E / Eh
-1.05
-1.10
-1.15
0.6
0.8
1
1.2
1.4
1.6
1.8
2
2.2
2.4
2.6
2.8
3
3.2
3.4
r(H-H) / Å


Potential energy curves for the dissociation of H2
field strength: 0.08 a.u.
E / Eh
r(H-H) / Å
-1.10
-1.15
-1.20
-1.25
-1.30
0.6
0.8
1
1.2
1.4
1.6
1.8
2
2.2
2.4
2.6
2.8
3
3.2
3.4
FCI
R-BLYP
R-LC-BLYP
R-B3LYP
R-CAM-B3LYP
R-B2LYP
R-B2PLYP
R-PBE
R-LC-PBE


Potential energy curves for the dissociation of H2
field strength: 0.08 a.u.
E / Eh
r(H-H) / Å
-1.10
-1.15
-1.20
-1.25
-1.30
0.6
0.8
1
1.2
1.4
1.6
1.8
2
2.2
2.4
2.6
2.8
3
3.2
3.4
FCI
U-BLYP
U-LC-BLYP
U-B3LYP
U-CAM-B3LYP
U-B2LYP
U-B2PLYP
U-PBE
U-LC-PBE


Potential energy curves for the dissociation of H2
field strength: 0.09 a.u.
E / Eh
r(H-H) / Å
-1.10
-1.15
-1.20
-1.25
-1.30
-1.35
0.6
0.8
1
1.2
1.4
1.6
1.8
2
2.2
2.4
2.6
2.8
3
3.2
3.4
FCI
R-BLYP
R-LC-BLYP
R-B3LYP
R-CAM-B3LYP
R-B2LYP
R-B2PLYP
R-PBE
R-LC-PBE


Potential energy curves for the dissociation of H2
field strength: 0.09 a.u.
E / Eh
r(H-H) / Å
-1.10
-1.15
-1.20
-1.25
-1.30
-1.35
0.6
0.8
1
1.2
1.4
1.6
1.8
2
2.2
2.4
2.6
2.8
3
3.2
3.4
FCI
U-BLYP
U-LC-BLYP
U-B3LYP
U-CAM-B3LYP
U-B2LYP
U-B2PLYP
U-PBE
U-LC-PBE