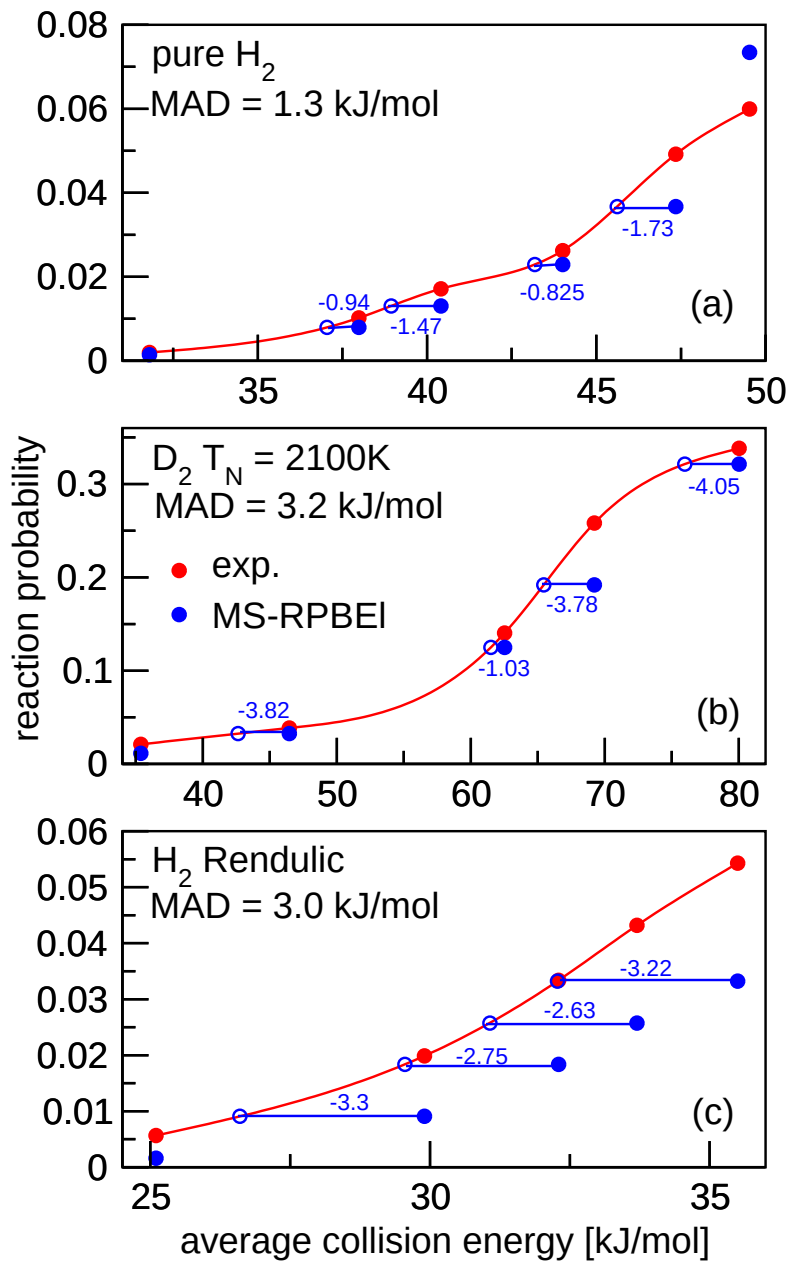
pure H_2
MAD = 1.3 kJ/mol
-0.94
-1.47
-0.825
-1.73
(a)
D_2 T_N = 2100K
MAD = 3.2 kJ/mol
exp.
MS-RPBEl
-3.82
-1.03
-3.78
-4.05
(b)
H_2 Rendulic
MAD = 3.0 kJ/mol
-3.3
-2.75
-2.63
-3.22
(c)
reaction probability
average collision energy [kJ/mol]