

Table S1. Energy values (Hartree) of $Fe - MP + nH_2$ ($n = 1 - 20$) frameworks. E_t is the total electronic energy; $E_t + E_{ZPE}$ is the sum of electronic and zero-point energies; $E_t + E_{thermal}$ is the sum of electronic and thermal energies; $H_{thermal}$ is the sum of electronic and thermal enthalpies; $G_{thermal}$ is the sum of electronic and thermal free energies.

nH_2	E_t	$E_t + E_{ZPE}$	$E_t + E_{thermal}$	$H_{thermal}$	$G_{thermal}$
0	-2252.1485	-2251.8705	-2251.8538	-2251.8528	-2251.9139
1	-2253.3497	-2253.0538	-2253.0360	-2253.0351	-2253.0978
2	-2254.5285	-2254.2209	-2254.1999	-2254.1990	-2254.2685
3	-2255.7073	-2255.3875	-2255.3634	-2255.3625	-2255.4384
4	-2256.8862	-2256.5550	-2256.5273	-2256.5264	-2256.6107
5	-2258.0649	-2257.7222	-2257.6911	-2257.6902	-2257.7818
6	-2259.2425	-2258.8880	-2258.8544	-2258.8534	-2258.9500
7	-2260.4201	-2260.0541	-2260.0169	-2260.0159	-2260.1213
8	-2261.5976	-2261.2191	-2261.1792	-2261.1783	-2261.2878
9	-2262.7754	-2262.3843	-2262.3413	-2262.3404	-2262.4570
10	-2263.9528	-2263.5494	-2263.5033	-2263.5024	-2263.6253
11	-2265.1404	-2264.7216	-2264.6744	-2264.6735	-2264.7974
12	-2266.3192	-2265.8879	-2265.8379	-2265.8370	-2265.9665
13	-2267.4977	-2267.0550	-2267.0015	-2267.0005	-2267.1380
14	-2268.6767	-2268.2216	-2268.1652	-2268.1642	-2268.3068
15	-2269.8556	-2269.3894	-2269.3292	-2269.3283	-2269.4793
16	-2271.0329	-2270.5538	-2270.4912	-2270.4903	-2270.6468
17	-2272.2103	-2271.7215	-2271.6571	-2271.6562	-2271.8170
18	-2273.3881	-2272.8848	-2272.8161	-2272.8152	-2272.9840
19	-2274.5659	-2274.0503	-2273.9784	-2273.9775	-2274.1526
20	-2275.7434	-2275.2157	-2275.1411	-2275.1402	-2275.3196