SUPPORTING INFORMATION

A DFT Study of Hydrogen Assisted Dissociation of CO By HCO, COH and HCOH Formation on Fe(100)

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Table S1. Adsorption energy of CO on top site on Fe(100) surface, calculated with equation 1 for a 4-layer slab varying the size of the supercell (See Figure S4).					
Size of supercell	CO/Fe – Top site (eV)	Fe Energy (eV)	CO energy (eV)	Adsorption energy (eV)	Magnetization μ_B /Fe-atom
Bulk	--	--	--	--	2.30
1x1	-3623.3188	-3033.922	-587.678	-1.718	2.24
2x2	-12726.210	-12136.610		**-1.922**	2.71
2x3	-18794.700	-18205.098		**-1.923**	2.63
3x3	-27896.198	-27306.573		**-1.947**	2.75
4x4	-49136.795	-48547.128		**-1.989**	2.68

Table S2. Adsorption energy of atomic hydrogen on Fe(100) hollow site, calculated with equation 1 varying the number of layers of the slab from 1 to 6.					
Number of layer slab	Total energy of Fe/H (eV)	H energy (eV)	Energy of the Fe slab (eV)	Adsorption energy (eV)	Magnetization μ_B /Fe-atom
Bulk	--	--	--	--	2.30
1	-3042.966	-12.553	-3023.964	-6.447	2.84
2	-6079.185		-6060.543	-6.088	2.81
3	-9114.815		-9099.214	-3.047	2.77
4	-12153.112		-12136.871	**-3.687**	2.71
5	-15190.026		-15173.775	**-3.697**	2.53
6	-18226.353		-18210.101	**-3.698**	2.64

Table S3. Adsorption energy of hydrogen on Fe(100) hollow site calculated with the magnetization per cell constrained to have $2.2\mu_{B/atom}$ and with the magnetization self-consistently calculated.						
Number of Fe atoms	Layers	Cell Magnetization Constrain ($2.2\ \mu_{B/atom}$)*(Number of Fe atoms)		Magnetization in the bare slab of Fe(100)	Not Magnetization Constrain (used in this Work)	
4	1	8.8 $\mu_{B/cell}$	-4.188	2.76 $\mu_{B/atom}$	2.84 $\mu_{B/atom}$	-6.447
8	2	17.6 $\mu_{B/cell}$	-3.871	2.43 $\mu_{B/atom}$	2.81 $\mu_{B/atom}$	-6.088
12	3	26.4 $\mu_{B/cell}$	-3.831	2.71 $\mu_{B/atom}$	2.77 $\mu_{B/atom}$	-3.047
16	**4**	**35.2 $\mu_{B/cell}$**	**-3.670**	2.60 $\mu_{B/atom}$	2.71 $\mu_{B/atom}$	**-3.687**
20	**5**	**44.0 $\mu_{B/cell}$**	**-3.996**	2.65 $\mu_{B/atom}$	2.53 $\mu_{B/atom}$	**-3.697**
24	**6**	**52.8 $\mu_{B/cell}$**	**-3.786**	2.64 $\mu_{B/atom}$	2.64 $\mu_{B/atom}$	**-3.698**

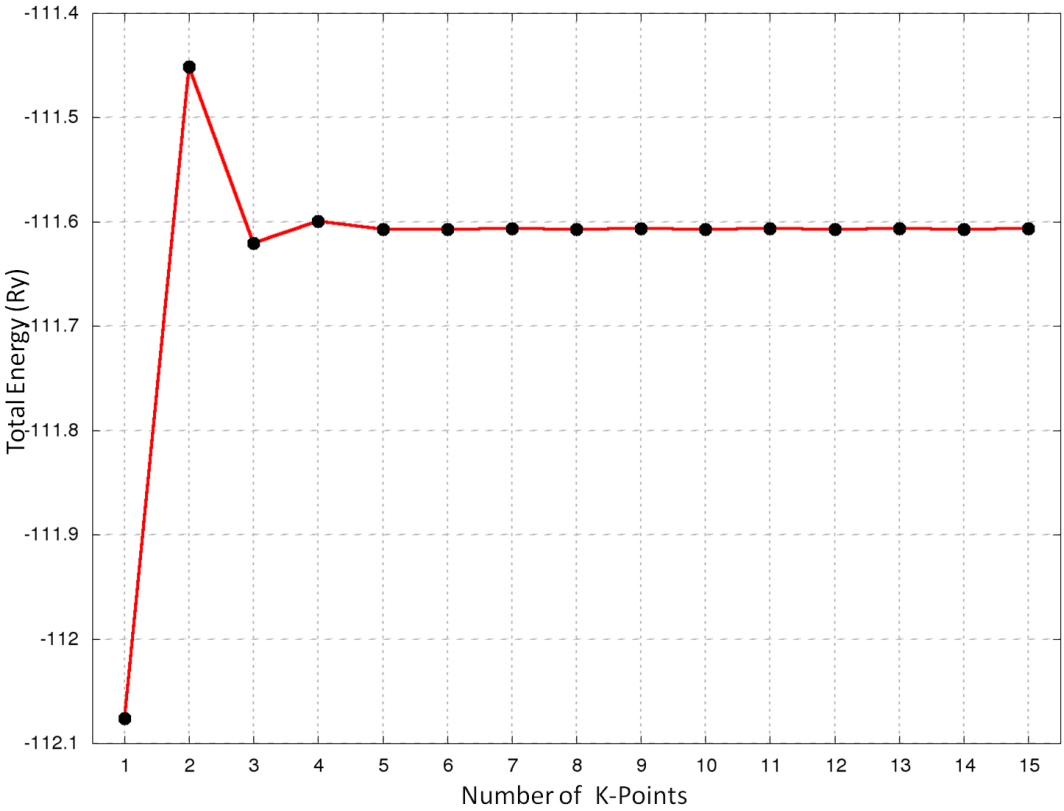

Figure S1. Convergence of the number of K-points calculated for Bulk Fe.

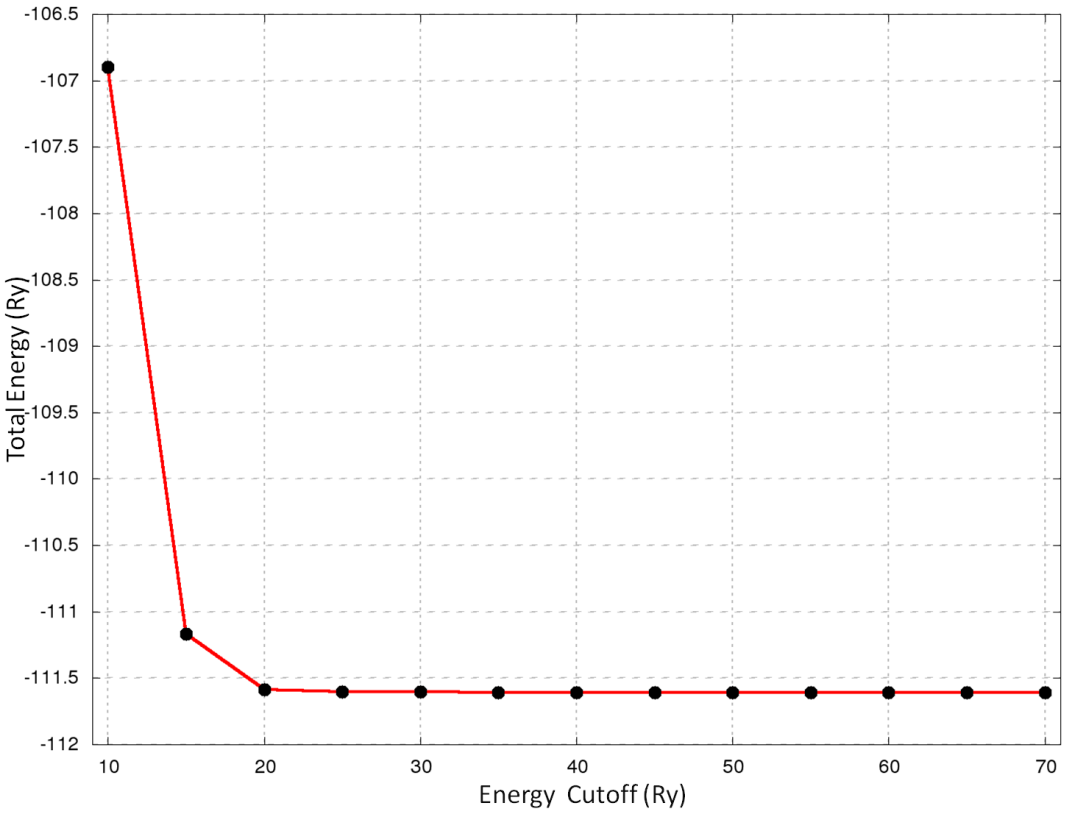

Figure S2. Convergence of the energy cutoff calculated for bulk Fe.

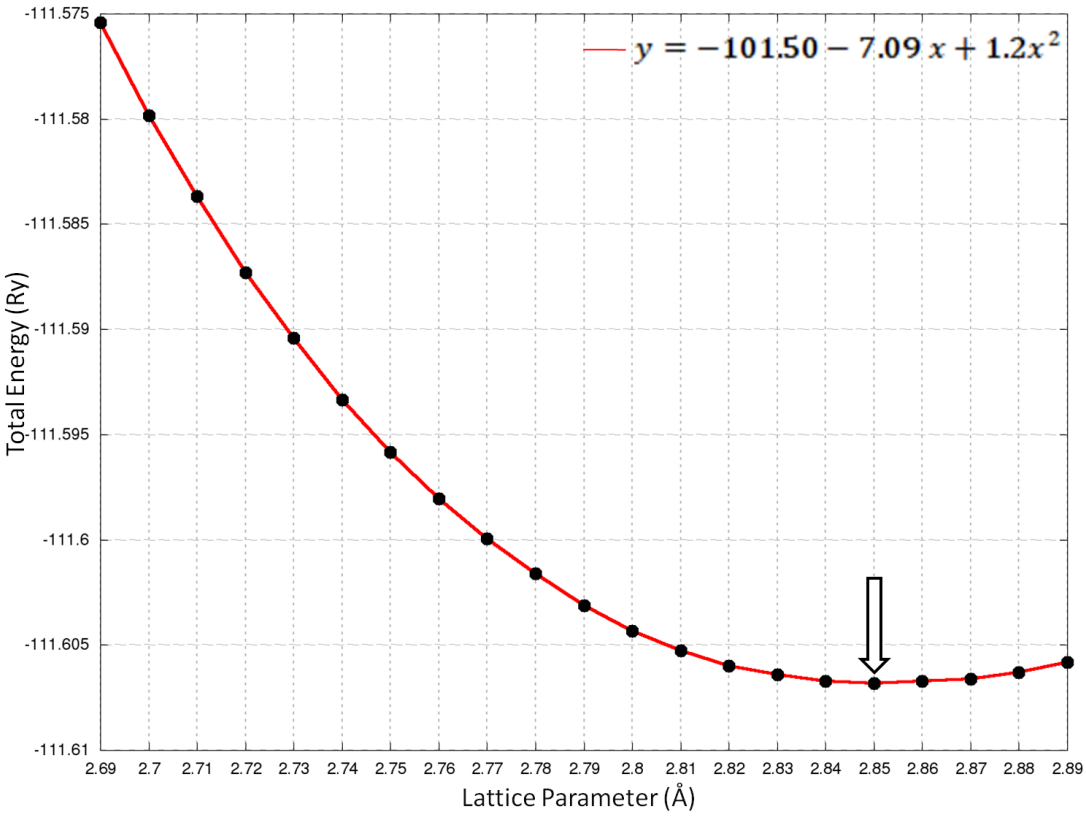

Figure S3. Lattice parameter of bulk Fe calculated in 2.85 Å.

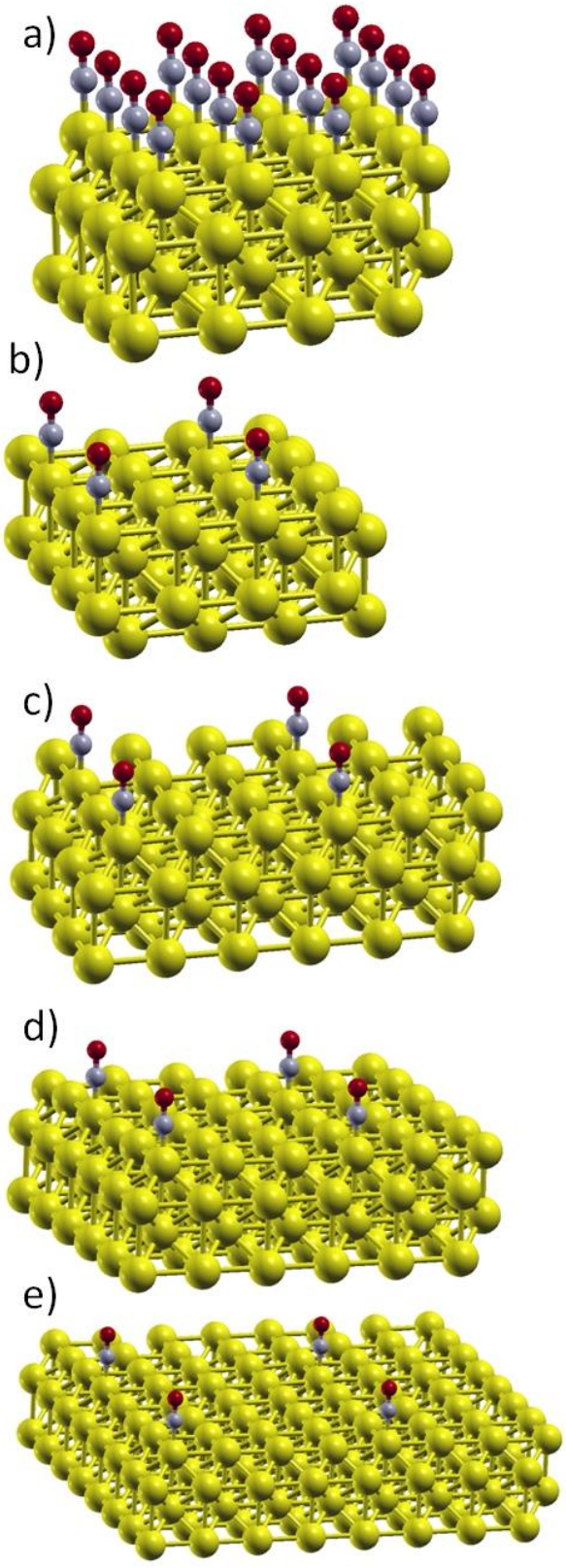

Figure S4. Adsorption of CO on top site for a Fe(100) surface varying the size of the supercell: a) (1x1) supercell, b) (2x2) supercell, c) (2x3) supercell, d) (3x3) supercell, e) (4x4) supercell.