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Surface Morphology Evolution of Cobalt Nanoparticle Induced by Hydrogen Adsorption: A Theoretical Study

Xiaobin Geng[a,c], Jinjia Liu[b,c,*], Hui Yang[b,c,d],Wenping Guo[c], Jie Bai[a,*] and Xiaodong Wen[b,c,*]

[a] *Inner Mongolia University of technology, Huhhot 010000, China*

[b] *State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan, 030001, China*

[c] *National Energy Center for Coal to Liquids, Synfuels China Co., Ltd, Huairou District, Beijing, 101400, China*

[d] *University of Chinese Academy of Sciences, No. 19A Yuquan Road, Beijing, 100049, China*

Corresponding Author:

Jinjia Liu (Email: liujj6636@163.com)

Jie Bai (Email: baijie@imut.edu.cn)

Xiao-Dong Wen (Email: wxd@sxicc.ac.cn)

Table S1. Calculated most stable H adsorption energy (E_{ads}, in eV), the most stable site of H adsorption on HCP-Co, the distance (d_{Co-H}, in Å) between the H atom and the cobalt surface.

Table S2. Surface energies (γ , in eV/Å^2) and surface area proportion Ss (%) of facets exposed on HCP-Co surfaces under H atmosphere at T = 300 K.

Table S3. Surface energies (γ , in eV/Å^2) and surface area proportion Ss (%) of facets exposed on HCP-Co surfaces under H atmosphere at T = 500 K.

Table S4. Surface energies (γ , in eV/Å^2) and surface area proportion Ss (%) of facets exposed on HCP-Co surfaces under H atmosphere at T= 700 K.

Figure S1. The structure of H adsorbed on Co(0001) before and after the optimization calculation.

Figure S2-7. Structures and stepwise adsorption energies ΔE (eV) of H atoms on six Co surfaces.

Figure S8. Change of Gibbs free energy of the Co (0001) (10-10) (10-11) (10-12) (11-20) (11-21) with nH atoms as a function of H_2 chemical potential

Table S1. Calculated most stable H adsorption energy (E_{ads}, in eV), the most stable site of adsorption H on HCP-Co, the distance (d_{Co-H}, in Å) between the H atom and the cobalt surface.

(hkil)	d_{Co-H} (Å)	site	E_{ads} (eV)
0001	0.964	f	-0.47
10-10	0.867	3f2	-0.56
10-11	0.897	3f2	-0.54
10-12	0.655	3f2	-0.53
11-20	1.110	bg1	-0.35
11-21	0.936	3f1	-0.50

Table S2. Surface energies (γ , in eV/Å^2) and surface area proportion Ss (%) of facets exposed on HCP-Co surfaces under H atmosphere at T = 300 K.

	1 atm		10 atm		20 atm		30 atm	
	γ (eV/Å^2)	Ss (%)	γ (eV/Å^2)	Ss (%)	γ (eV/Å^2)	Ss (%)	γ (eV/Å^2)	Ss (%)
Co (0001)	0.101	15	0.097	15	0.095	15	0.094	15
Co (10-10)	0.102	16	0.096	17	0.094	17	0.093	17
Co (10-11)	0.098	69	0.093	68	0.091	68	0.090	68
Co (10-12)	0.115	0	0.110	0	0.108	0	0.108	0
Co (11-20)	0.149	0	0.144	0	0.141	0	0.140	0
Co (11-21)	0.138	0	0.133	0	0.132	0	0.131	0

Table S3. Surface energies (γ , in eV/Å^2) and surface area proportion Ss (%) of facets exposed on HCP-Co surfaces under H atmosphere at T = 500 K.

	1 atm		10 atm		20 atm		30 atm	
	γ (eV/Å^2)	Ss (%)	γ (eV/Å^2)	Ss (%)	γ (eV/Å^2)	Ss (%)	γ (eV/Å^2)	Ss (%)
Co (0001)	0.121	14	0.114	15	0.112	15	0.111	15
Co (10-10)	0.130	14	0.121	11	0.118	12	0.117	12
Co (10-11)	0.123	65	0.114	70	0.112	70	0.110	71
Co (10-12)	0.135	7	0.128	4	0.126	3	0.125	2
Co (11-20)	0.157	0	0.157	0	0.157	0	0.157	0
Co (11-21)	0.154	0	0.149	0	0.147	0	0.147	0

Table S4. Surface energies (γ , in eV/Å^2) and surface area proportion Ss (%) of facets exposed on HCP-Co surfaces under H atmosphere at T = 700 K.

	1 atm		10 atm		20 atm		30 atm	
	γ (eV/Å^2)	Ss (%)	γ (eV/Å^2)	Ss (%)	γ (eV/Å^2)	Ss (%)	γ (eV/Å^2)	Ss (%)
Co (0001)	0.132	17	0.130	14	0.128	14	0.127	14
Co (10-10)	0.141	26	0.139	20	0.137	20	0.136	18
Co (10-11)	0.147	42	0.138	51	0.135	53	0.132	58
Co (10-12)	0.156	11	0.147	13	0.144	13	0.143	10
Co (11-20)	0.157	4	0.157	2	0.157	0	0.157	0
Co (11-21)	0.165	0	0.161	0	0.160	0	0.159	0

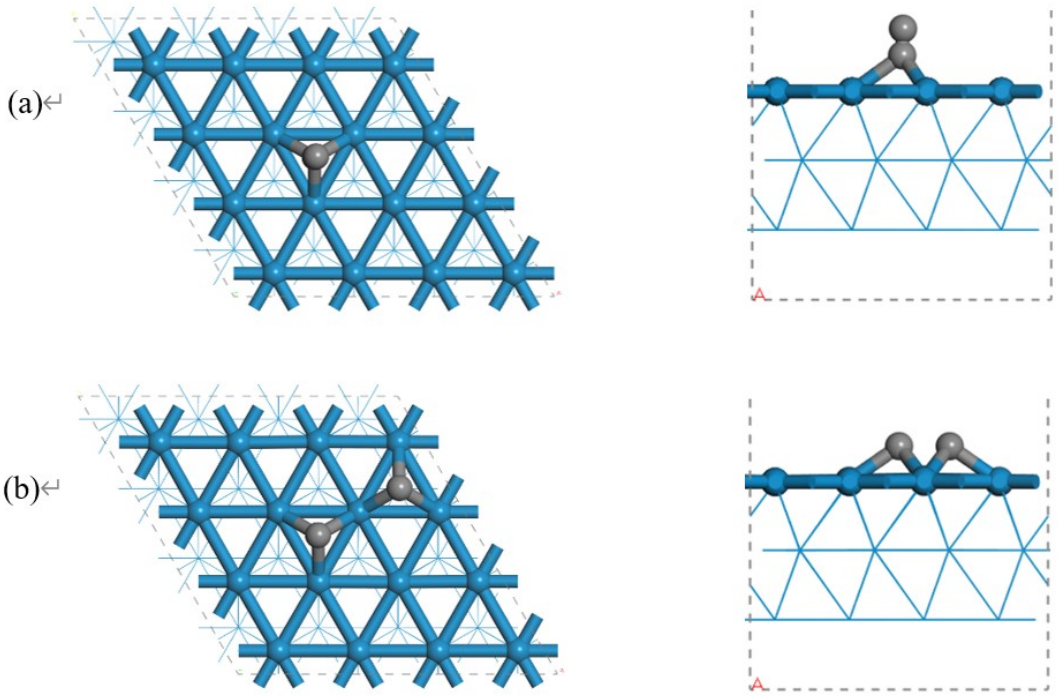

Figure S1. The structure of H adsorbed on Co (0001) before (a) and after (b) the optimization calculation. (Gray is hydrogen atom, blue is cobalt atom)

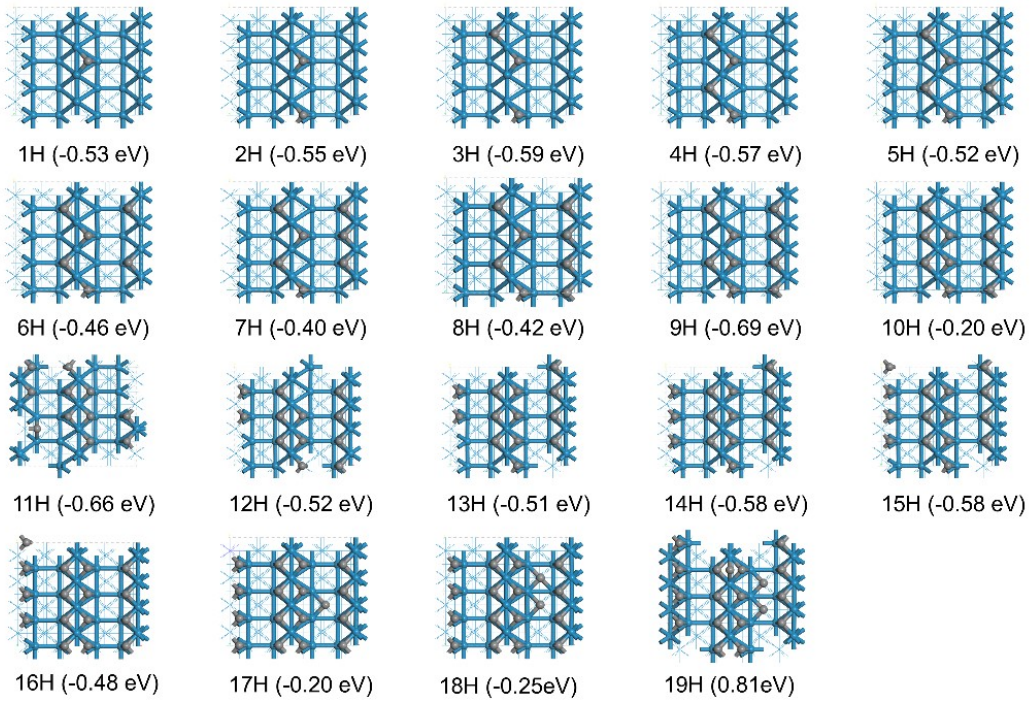

Figure S2. Structures and stepwise adsorption energies ΔE_{ads} (eV) of n_H atoms on Co (10-12). (Gray is hydrogen atom, blue is cobalt atom)

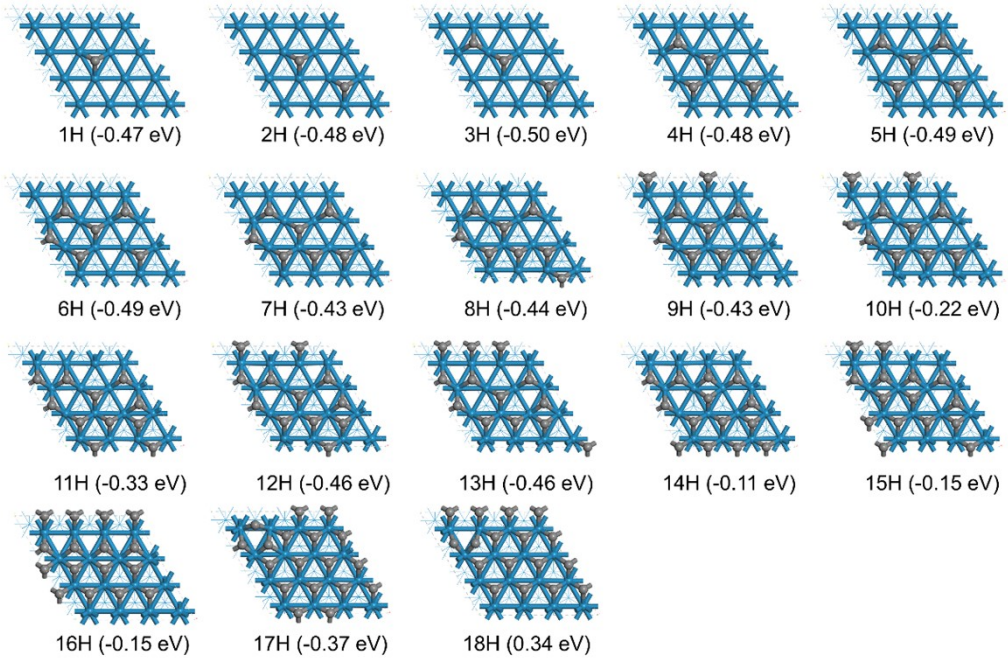

Figure S3. Structures and stepwise adsorption energies ΔE_{ads} (eV) of n_H atoms on Co (0001). (Gray is hydrogen atom, blue is cobalt atom)

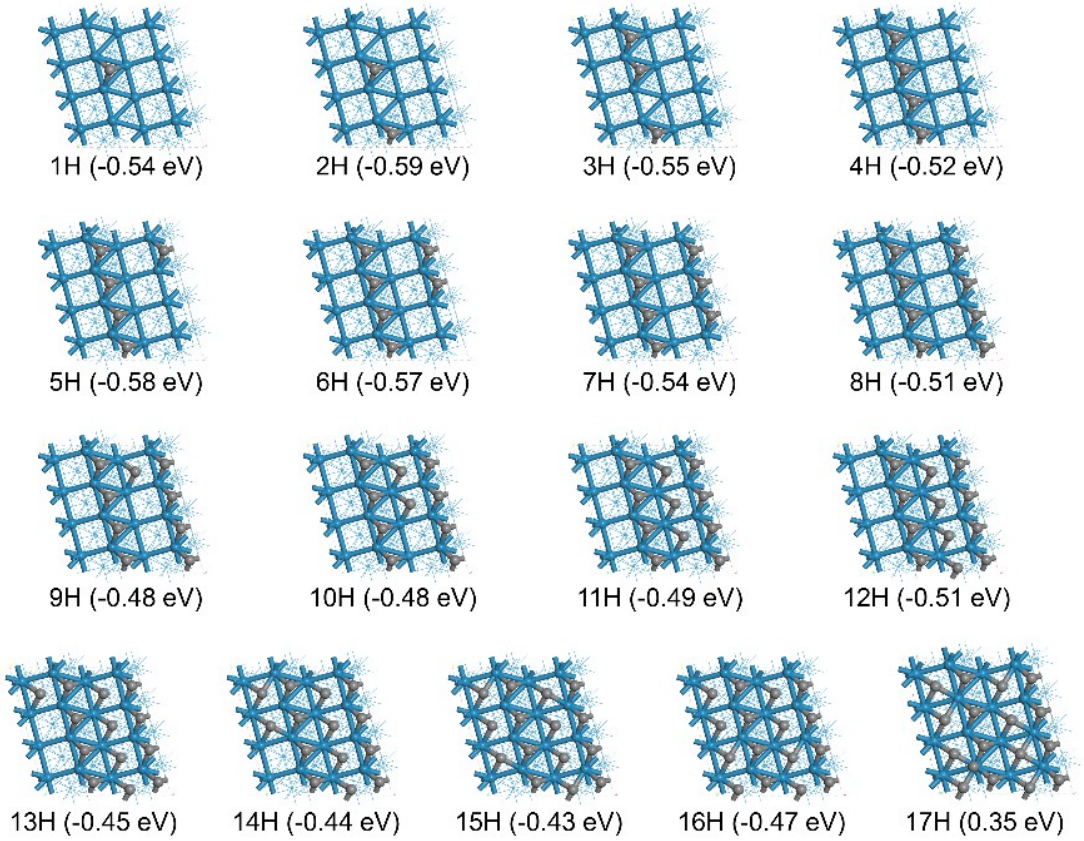

Figure S4. Structures and stepwise adsorption energies ΔE_{ads} (eV) of n_H atoms on Co (10-11). (Gray is hydrogen atom, blue is cobalt atom)

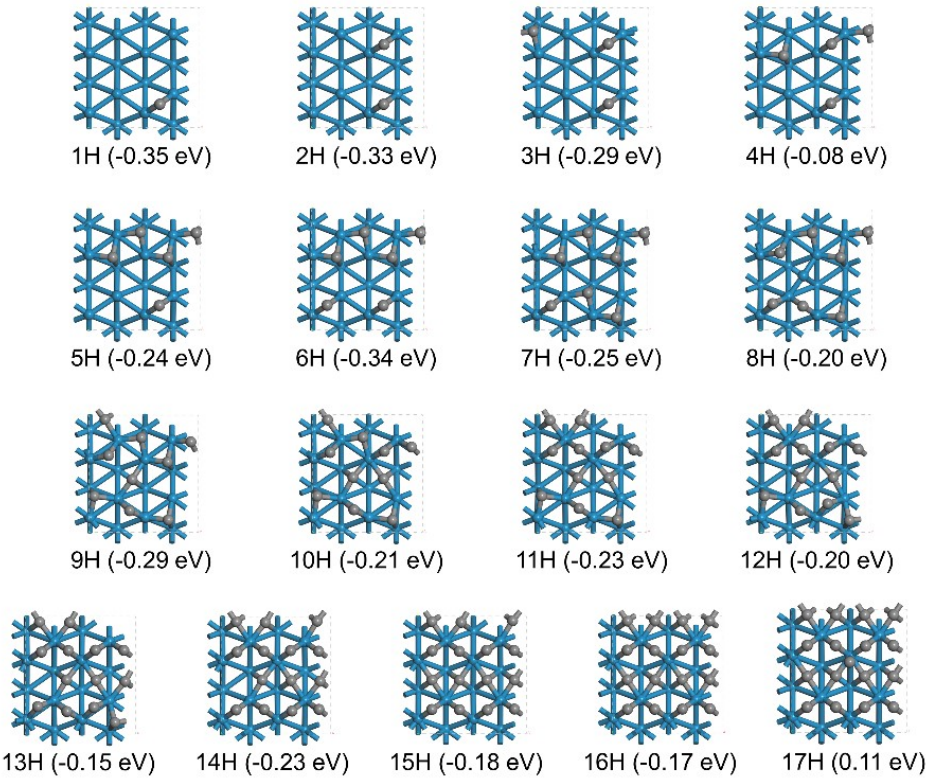

Figure S5. Structures and stepwise adsorption energies ΔE_{ads} (eV) of n_H atoms on Co (11-20). (Gray is hydrogen atom, blue is cobalt atom)

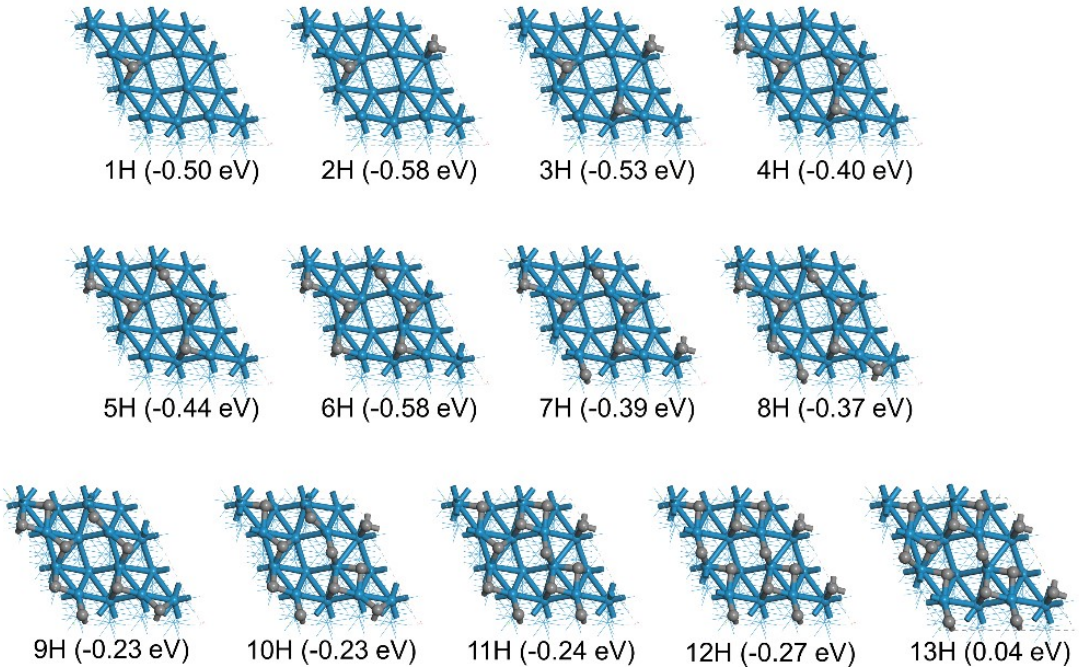

Figure S6. Structures and stepwise adsorption energies ΔE_{ads} (eV) of n_H atoms on Co (11-21). (Gray is hydrogen atom, blue is cobalt atom)

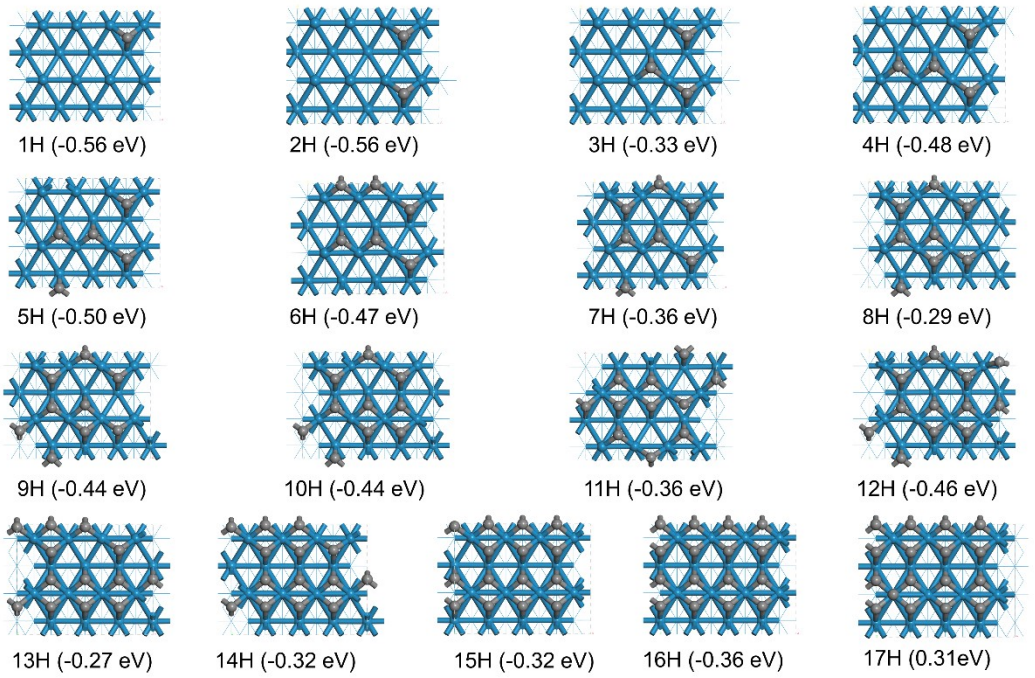

Figure S7. Structures and stepwise adsorption energies ΔE_{ads} (eV) of n_H atoms on Co (10-10). (Gray is hydrogen atom, blue is cobalt atom)

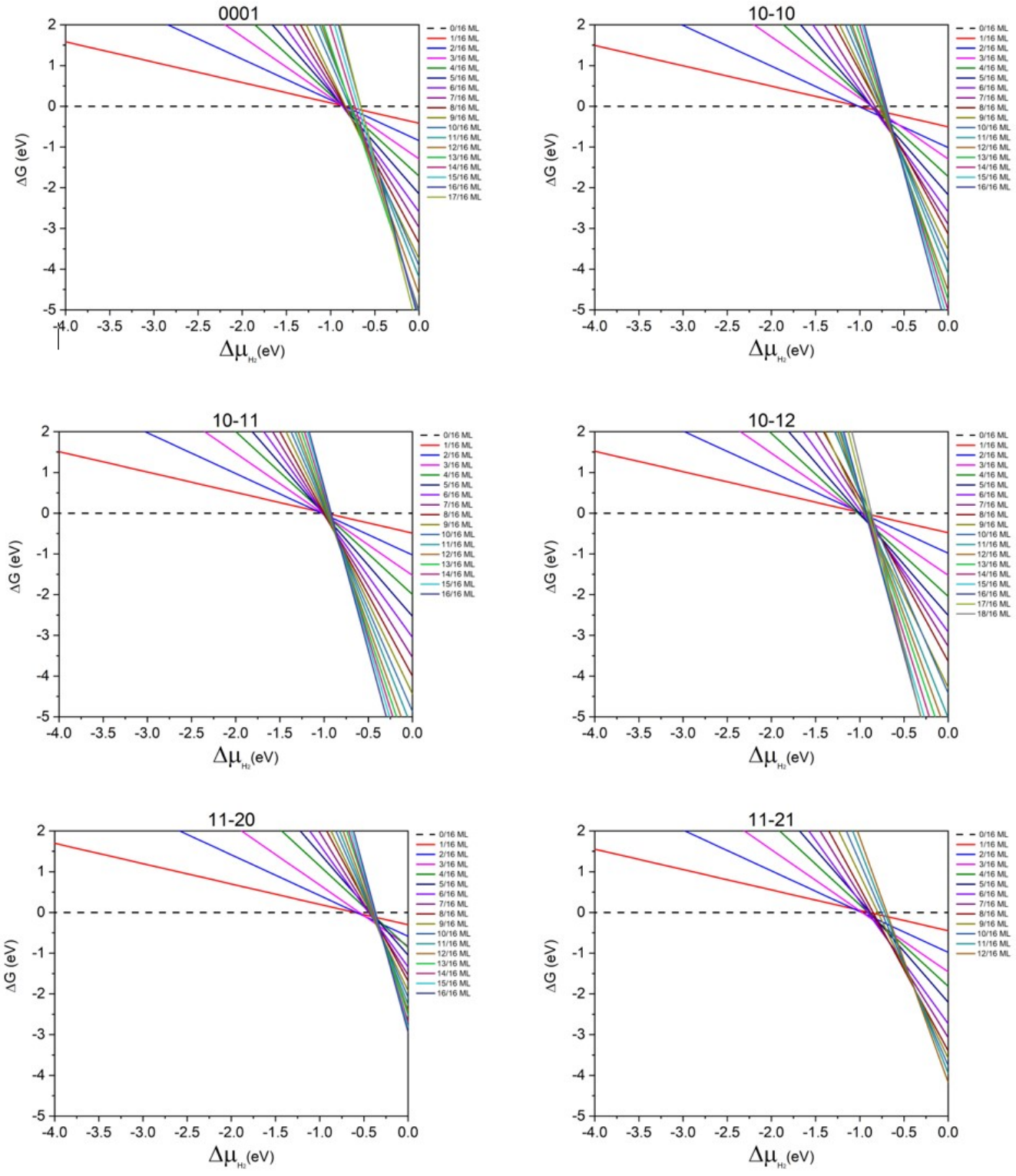

Figure S8. Change of Gibbs free energy of the Co (0001) (10-10) (10-11) (10-12) (11-20) (11-21) with n_H atoms as a function of H_2 chemical potential