Supplementary material

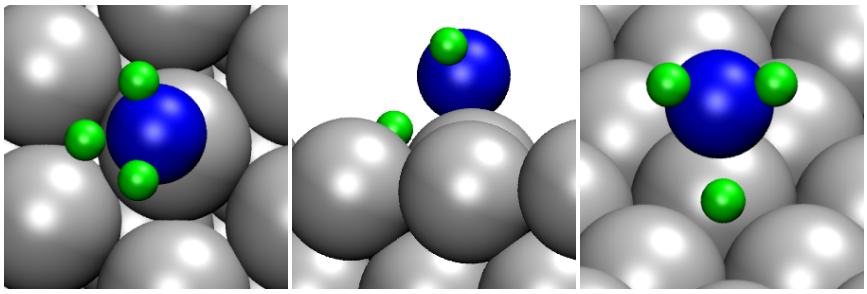


Figure S1: The transition state for the first dehydrogenation step for ammonia dehydrogenation process on a late transition metal close packed surface. The hydrogen atom moves towards the nearest hollow site and NH_2 is staying on a on top site. Colors for the atoms; green is hydrogen, blue is nitrogen and gray atoms are the transition metal.

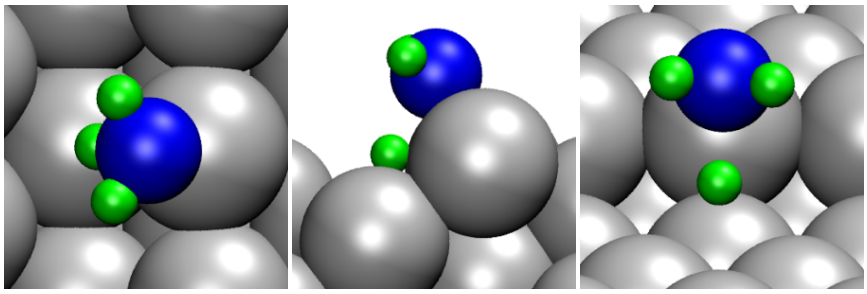


Figure S2: The transition state for the first dehydrogenation step for ammonia dehydrogenation process on a late transition metal stepped surface. The hydrogen atom moves towards the nearest on top site on the terrace below and NH_2 is staying at the top of the step edge on a on top site. Colors for the atoms; green is hydrogen, blue is nitrogen and gray atoms are the transition metal.

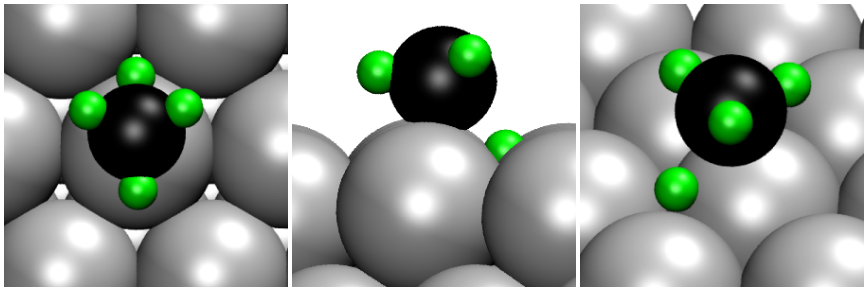


Figure S3: The transition state for the first dehydrogenation step for methane dehydrogenation process on a late transition metal close packed surface. The hydrogen atom moves towards the nearest hollow site and CH_3 is staying on a on top site. Colors for the atoms; green are hydrogen, black is carbon and gray atoms are the transition metal.

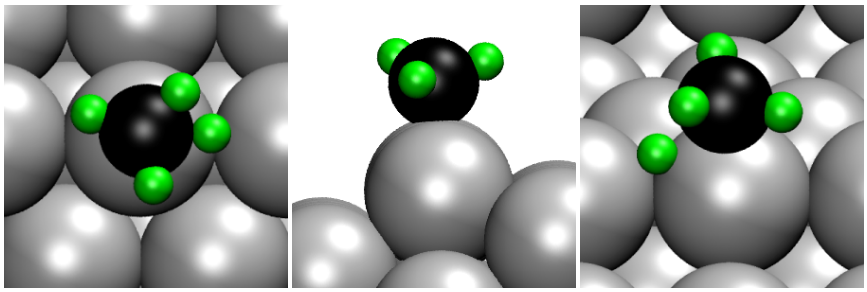


Figure S4: The transition state for the first dehydrogenation step for the methane dehydrogenation process on a late transition metal stepped surface. The hydrogen atom moves towards the nearest bridge on the step edge and CH_3 is staying at the top of the step edge on a on top site. Colors for the atoms; green is hydrogen, black is carbon and gray atoms are the transition metal.

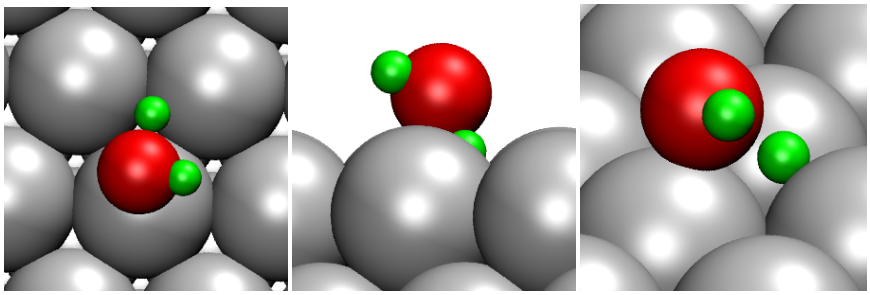


Figure S5: The transition state for the first dehydrogenation step for water dehydrogenation process on a late transition metal close packed surface. The hydrogen atom moves towards the nearest bridge site and OH is staying on a on top site. Colors for the atoms; green are hydrogen, red is oxygen and gray atoms are the transition metal.

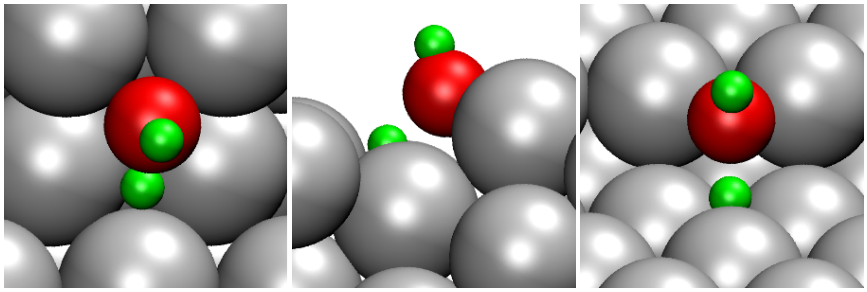
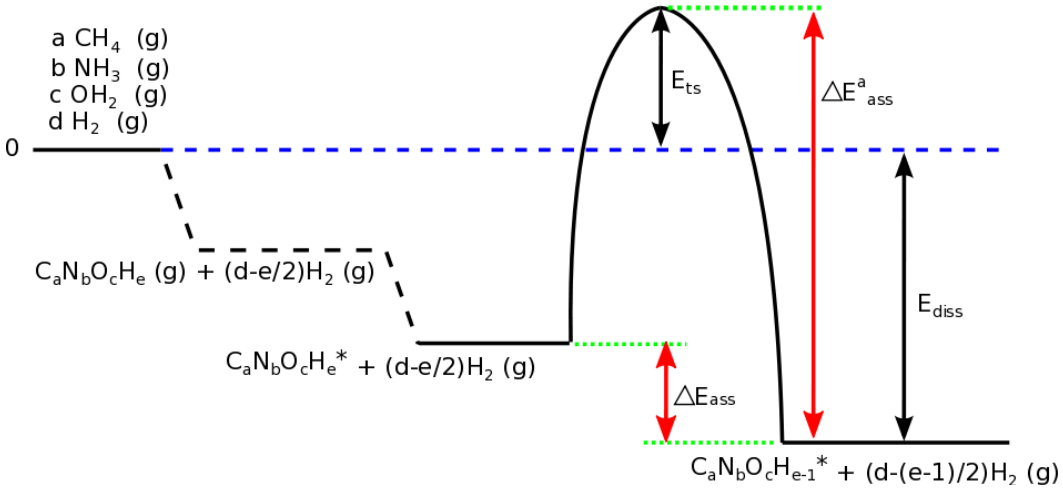
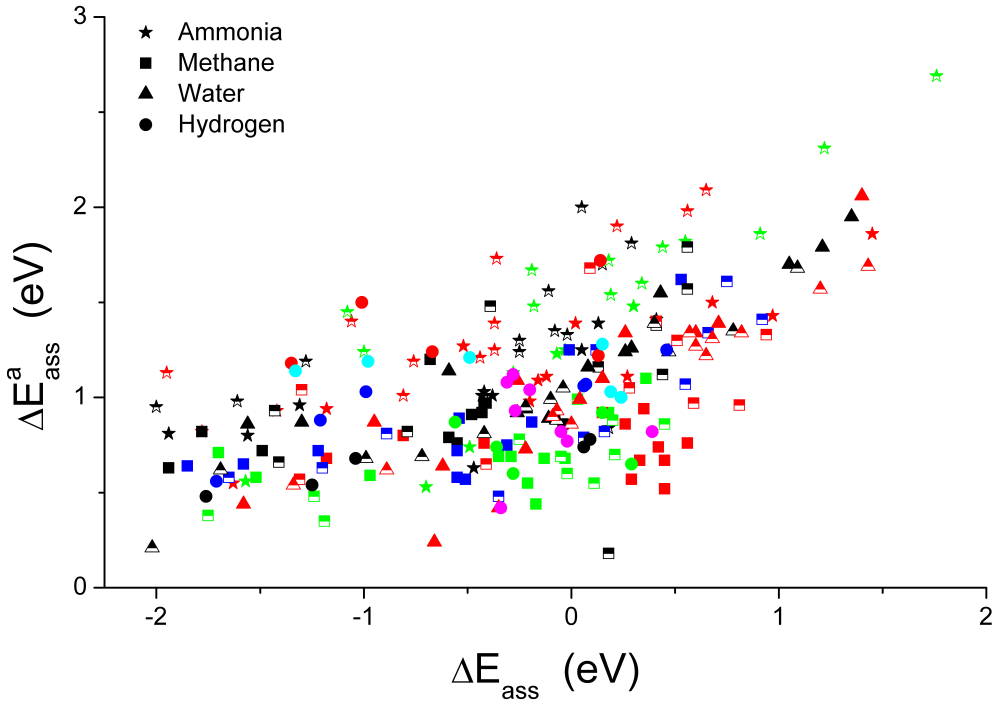


Figure S6: The transition state for the first dehydrogenation step for the water dehydrogenation process on a late transition metal stepped surface. The hydrogen atom moves towards a hollow site on the step edge and OH is staying at the bridge site on the front of the step edge. Colors for the atoms; green is hydrogen, red is oxygen and gray atoms are the transition metal.



S7: The energy diagram used to define the energies of the system for the hydrogenation processes.



S8: The BEP relation for the hydrogenation reaction.

Reaction	*Model system*	*Layers*	*Relaxed Layers*	*k-point sampling*	*Planewave cutoff [eV]*	*Density cutoff [eV]*	*Vacuum (x,y,z) [Å]*	*Surface unitcells*	*Quasi Newton force [eV / Å]*
OO-dehydrogenation	M12	2	0	(1,1,1)	408	816	(10,10,10)	N/A	0.05
Ammonia dehydrogenation	(211)	9	6	(4,4,1)	350	700	(0,0,10)	1 x 2	0.05
Ammonia dehydrogenation	(111)	3	1	(4,4,1)	350	700	(0,0,10)	2 x 2	0.05
Water	(211)	9	3	(4,4,1)	340	680	(0,0,10)	1 x 2	0.05
	(111)	3	1	(4,4,1)	340	680	(0,0,10)	2 x 2	0.05
CHx	(211)	9	6	(4,4,1)	340	500	(0,0,10)	1 x 3	0.05
	(111)	3	1	(4,4,1)	340	500	(0,0,10)	2 x 2	0.05
CyHx	(211)	9	3	(4,4,1)	350	700	(0,0,10)	2 x 3	0.05
Hydrogen	(211)	9	3	(4,4,1)	350	700	(0,0,10-12)	2 x 3	0.05
	(111)	3	1	(4,4,1)	350	700	(0,0,10-12)	2 x 2	0.05

TS1: The parameters used in the calculations for the different dehydrogenation reactions.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$H_2O^* \rightarrow OH^* + H^*$	(111)	Au	-0.026	1.997	1.558
$H_2O^* \rightarrow OH^* + H^*$	(111)	Ag	-0.041	1.783	0.914
$H_2O^* \rightarrow OH^* + H^*$	(111)	Pt	-0.051	0.849	0.605
$H_2O^* \rightarrow OH^* + H^*$	(111)	Pd	-0.081	1.182	0.542
$H_2O^* \rightarrow OH^* + H^*$	(111)	Re	-0.165	0.515	-0.875
$H_2O^* \rightarrow OH^* + H^*$	(111)	Ir	-0.091	0.679	0.262
$H_2O^* \rightarrow OH^* + H^*$	(111)	Ru	-0.207	0.739	-0.25
$H_2O^* \rightarrow OH^* + H^*$	(111)	Rh	-0.105	0.845	0.111
$H_2O^* \rightarrow OH^* + H^*$	(111)	Cu	-0.041	1.303	0.215
$H_2O^* \rightarrow OH^* + H^*$	(111)	Ni	-0.046	0.909	-0.193
$H_2O^* \rightarrow OH^* + H^*$	(111)	Co	-0.054	1.026	-0.315
$H_2O^* \rightarrow OH^* + H^*$	(111)	Mn	-0.111	0.552	-1.506
$H_2O^* \rightarrow OH^* + H^*$	(111)	Fe	-0.092	0.651	-0.693

TS2 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$H_2O^* \rightarrow OH^* + H^*$	(211)	Au	-0.061	1.82	1.278
$H_2O^* \rightarrow OH^* + H^*$	(211)	Ag	-0.12	1.389	0.769
$H_2O^* \rightarrow OH^* + H^*$	(211)	Pt	-0.138723	0.719	-0.138
$H_2O^* \rightarrow OH^* + H^*$	(211)	Pd	-0.175283	0.823	-0.107
$H_2O^* \rightarrow OH^* + H^*$	(211)	Re	-0.575		-2.05
$H_2O^* \rightarrow OH^* + H^*$	(211)	Ir	-0.281	0.242	-1.1
$H_2O^* \rightarrow OH^* + H^*$	(211)	Ru	-0.569	-0.005	-1.22
$H_2O^* \rightarrow OH^* + H^*$	(211)	Rh	-0.284661	0.487	-0.857
$H_2O^* \rightarrow OH^* + H^*$	(211)	Cu	-0.184	0.798	-0.097
$H_2O^* \rightarrow OH^* + H^*$	(211)	Ni	-0.321	0.349	-0.921
$H_2O^* \rightarrow OH^* + H^*$	(211)	Co	-0.367	0.266	-1.043
$H_2O^* \rightarrow OH^* + H^*$	(211)	Mn	-0.509	-0.25	-1.943
$H_2O^* \rightarrow OH^* + H^*$	(211)	Fe	-0.515	-0.15	-1.716

TS3 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$OH^* \rightarrow O^* + H^*$	(111)	Au	1.388	3.563	2.691
$OH^* \rightarrow O^* + H^*$	(111)	Ag	0.67	3.092	2.235
$OH^* \rightarrow O^* + H^*$	(111)	Pt	0.957	2.118	1.177
$OH^* \rightarrow O^* + H^*$	(111)	Pd	0.937	2.117	1.198
$OH^* \rightarrow O^* + H^*$	(111)	Re	-0.349	0.251	-1.702
$OH^* \rightarrow O^* + H^*$	(111)	Ir	0.485	1.485	0.596
$OH^* \rightarrow O^* + H^*$	(111)	Ru	0.189	1.308	-0.239
$OH^* \rightarrow O^* + H^*$	(111)	Rh	0.431	1.515	0.353
$OH^* \rightarrow O^* + H^*$	(111)	Cu	0.303	2.032	0.897
$OH^* \rightarrow O^* + H^*$	(111)	Ni	0.198	1.176	-0.064
$OH^* \rightarrow O^* + H^*$	(111)	Co	0.045	1.015	-0.249
$OH^* \rightarrow O^* + H^*$	(111)	Mn	-0.852	-0.272	-2.063
$OH^* \rightarrow O^* + H^*$	(111)	Fe	-0.136	0.514	-1.184

TS4 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
OH* -> O* + H*	(211)	Au	0.939	3.175	2.962
OH* -> O* + H*	(211)	Ag	0.492	2.801	2.178
OH* -> O* + H*	(211)	Pt	0.362	1.6	0.786
OH* -> O* + H*	(211)	Pd	0.343	1.753	1.068
OH* -> O* + H*	(211)	Re	-1.364	-0.791	-2.141
OH* -> O* + H*	(211)	Ir	-0.396	0.596	-0.792
OH* -> O* + H*	(211)	Ru	-0.688	0.267	-0.617
OH* -> O* + H*	(211)	Rh	-0.365	0.729	-0.321
OH* -> O* + H*	(211)	Cu	-0.038	1.628	0.95
OH* -> O* + H*	(211)	Ni	-0.496	0.678	-0.275
OH* -> O* + H*	(211)	Co	-0.641	0.444	-0.542
OH* -> O* + H*	(211)	Mn	-1.277	-0.686	-2.368
OH* -> O* + H*	(211)	Fe	-1.12	-0.351	-1.588

TS5 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$NH_3^* \rightarrow NH_2^* + H^*$	(111)	Cu	-0.11		0.43
$NH_3^* \rightarrow NH_2^* + H^*$	(111)	Re	-0.55	0.63	-0.85
$NH_3^* \rightarrow NH_2^* + H^*$	(111)	Mo		-0.19	-2.46
$NH_3^* \rightarrow NH_2^* + H^*$	(111)	Ru	-0.56		-0.43
$NH_3^* \rightarrow NH_2^* + H^*$	(111)	Rh	-0.49	0.92	-0.21
$NH_3^* \rightarrow NH_2^* + H^*$	(111)	Co	-1.45	-0.14	-1.37
$NH_3^* \rightarrow NH_2^* + H^*$	(111)	Ir	-0.62	0.6	-0.14
$NH_3^* \rightarrow NH_2^* + H^*$	(111)	Ni	-0.25	1.03	-0.22
$NH_3^* \rightarrow NH_2^* + H^*$	(111)	Pt	-0.56	0.67	0.14
$NH_3^* \rightarrow NH_2^* + H^*$	(111)	Pd	-0.4		0.2
$NH_3^* \rightarrow NH_2^* + H^*$	(111)	Au	-0.07		1.47
$NH_3^* \rightarrow NH_2^* + H^*$	(111)	Ag	-0.08		1.23
$NH_3^* \rightarrow NH_2^* + H^*$	(111)	Os			-0.58
$NH_3^* \rightarrow NH_2^* + H^*$	(111)	Cd	-0.07	2.06	1.5
$NH_3^* \rightarrow NH_2^* + H^*$	(111)	Fe	-0.67		-1.11
$NH_3^* \rightarrow NH_2^* + H^*$	(111)	Mn	-0.38		-1.09

TS6 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$NH_3^* \rightarrow NH_2^* + H^*$	(211)	Cu	-0.41	1.24	-0.23
$NH_3^* \rightarrow NH_2^* + H^*$	(211)	Re	-0.98	-0.02	-1.89
$NH_3^* \rightarrow NH_2^* + H^*$	(211)	Mo	-1.15	-0.06	-2.37
$NH_3^* \rightarrow NH_2^* + H^*$	(211)	Ru	-0.97	0.3	-1.3
$NH_3^* \rightarrow NH_2^* + H^*$	(211)	Rh	-0.7	0.65	-0.89
$NH_3^* \rightarrow NH_2^* + H^*$	(211)	Ir	-0.95	0.31	-1.5
$NH_3^* \rightarrow NH_2^* + H^*$	(211)	Pt	-0.85	0.69	-1.03
$NH_3^* \rightarrow NH_2^* + H^*$	(211)	Pd	-0.61	1.25	-0.42
$NH_3^* \rightarrow NH_2^* + H^*$	(211)	Au	-0.29	1.95	0.71
$NH_3^* \rightarrow NH_2^* + H^*$	(211)	Ag	-0.25	2.28	0.83
$NH_3^* \rightarrow NH_2^* + H^*$	(211)	Cd	-0.17		0.91
$NH_3^* \rightarrow NH_2^* + H^*$	(211)	W	-1.34	-0.41	-3.1
$NH_3^* \rightarrow NH_2^* + H^*$	(211)	Mn	-0.81	0.25	
$NH_3^* \rightarrow NH_2^* + H^*$	(211)	Ni	-0.62	0.72	-1.07

TS7 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$NH_2^* \rightarrow NH^* + H^*$	(111)	Cu	0.52	2.31	1.05
$NH_2^* \rightarrow NH^* + H^*$	(111)	Re	-0.32	0.49	-1.01
$NH_2^* \rightarrow NH^* + H^*$	(111)	Mo	-1.16	-0.75	-2.61
$NH_2^* \rightarrow NH^* + H^*$	(111)	Ru	0.01	1.24	0.13
$NH_2^* \rightarrow NH^* + H^*$	(111)	Rh	0.12		0.17
$NH_2^* \rightarrow NH^* + H^*$	(111)	Co	-1.01		-1.28
$NH_2^* \rightarrow NH^* + H^*$	(111)	Ir	0.09	1.33	0.25
$NH_2^* \rightarrow NH^* + H^*$	(111)	Ni	0.18	1.02	-0.09
$NH_2^* \rightarrow NH^* + H^*$	(111)	Pt	0.48	1.86	0.47
$NH_2^* \rightarrow NH^* + H^*$	(111)	Pd	0.59	1.76	0.78
$NH_2^* \rightarrow NH^* + H^*$	(111)	Au	1.29	3.41	2.47
$NH_2^* \rightarrow NH^* + H^*$	(111)	Ag	0.99	3.35	2.41
$NH_2^* \rightarrow NH^* + H^*$	(111)	Os	-0.16		-0.35
$NH_2^* \rightarrow NH^* + H^*$	(111)	Cd	0.76	2.93	2.38
$NH_2^* \rightarrow NH^* + H^*$	(111)	Fe	-0.4		-1.29
$NH_2^* \rightarrow NH^* + H^*$	(111)	Mn	-0.42	0.04	-1.4

TS8 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$NH_2^* \rightarrow NH^* + H^*$	(211)	Cu	-0.09	2.37	0.97
$NH_2^* \rightarrow NH^* + H^*$	(211)	Re	-1.39	0.28	-1.62
$NH_2^* \rightarrow NH^* + H^*$	(211)	Mo	-1.45	-0.03	-2.01
$NH_2^* \rightarrow NH^* + H^*$	(211)	Ru	-0.86	0.89	-0.49
$NH_2^* \rightarrow NH^* + H^*$	(211)	Rh	-0.56	1.1	-0.12
$NH_2^* \rightarrow NH^* + H^*$	(211)	Ir	-0.87	1.22	-0.51
$NH_2^* \rightarrow NH^* + H^*$	(211)	Pt	-0.46	1.35	0.34
$NH_2^* \rightarrow NH^* + H^*$	(211)	Pd	-0.02	1.93	0.74
$NH_2^* \rightarrow NH^* + H^*$	(211)	Au	0.63	3.23	2.41
$NH_2^* \rightarrow NH^* + H^*$	(211)	Ag	0.58	3.65	2.53
$NH_2^* \rightarrow NH^* + H^*$	(211)	Cd	0.34		2.02
$NH_2^* \rightarrow NH^* + H^*$	(211)	W	-2.03	-0.6	-2.68
$NH_2^* \rightarrow NH^* + H^*$	(211)	Mn			-1.86
$NH_2^* \rightarrow NH^* + H^*$	(211)	Ni	-0.64	0.98	-0.27

TS9 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
NH* -> N* + H*	(111)	Cu	1.13	3.41	2.45
NH* -> N* + H*	(111)	Re	-0.48	0.72	-0.53
NH* -> N* + H*	(111)	Mo	-1.3	2.18	
NH* -> N* + H*	(111)	Ru	0.57		0.86
NH* -> N* + H*	(111)	Rh	0.5		0.8
NH* -> N* + H*	(111)	Co	-0.92	0.47	-0.54
NH* -> N* + H*	(111)	Ir	0.47	1.56	0.94
NH* -> N* + H*	(111)	Ni	0.3	1.74	0.73
NH* -> N* + H*	(111)	Pt	0.81	4.91	1.3
NH* -> N* + H*	(111)	Pd	1.17	2.62	1.59
NH* -> N* + H*	(111)	Au	2.29	4.65	3.85
NH* -> N* + H*	(111)	Ag	2.17	4.92	4.11
NH* -> N* + H*	(111)	Os	0.06		0.2
NH* -> N* + H*	(111)	Cd	1.64		3.88
NH* -> N* + H*	(111)	Fe	-0.58		-0.99
NH* -> N* + H*	(111)	Mn	-0.73	0.52	-0.87

TS10 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
NH* -> N* + H*	(211)	Cu	1.12	3.59	2.4
NH* -> N* + H*	(211)	Re	-1.13	-0.46	-1.3
NH* -> N* + H*	(211)	Mo	-1.1	0.85	-1.15
NH* -> N* + H*	(211)	Ru	-0.05	1.39	0.03
NH* -> N* + H*	(211)	Rh	0.22	1.57	0.24
NH* -> N* + H*	(211)	Ir	0.13	1.68	-0.02
NH* -> N* + H*	(211)	Pt	0.91	2.58	1.02
NH* -> N* + H*	(211)	Pd	1.15	2.69	1.39
NH* -> N* + H*	(211)	Au	2.32	4.91	3.93
NH* -> N* + H*	(211)	Ag	2.27	5.22	4.27
NH* -> N* + H*	(211)	Cd	1.44		3.26
NH* -> N* + H*	(211)	W	-1.62	-0.62	-2.03
NH* -> N* + H*	(211)	Mn	-1.2	0.32	-1.49
NH* -> N* + H*	(211)	Ni	0.16	1.66	0.42

TS11 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
CH_4* -> CH_3* + H*	(111)	Pt	0	1.06	0.19
CH_4* -> CH_3* + H*	(111)	Pd	0	1.13	0.55
CH_4* -> CH_3* + H*	(111)	Ru	0	1.06	0.31
CH_4* -> CH_3* + H*	(111)	Re	0	1.25	0.01
CH_4* -> CH_3* + H*	(111)	Co	0	1.43	0.54
CH_4* -> CH_3* + H*	(111)	Ni	0	1.27	0.55
CH_4* -> CH_3* + H*	(111)	Mn	0	1.09	-0.53
CH_4* -> CH_3* +	(111)	Cu	0	1.94	1.22

H^*					
$CH_4^* \rightarrow CH_3^* + H^*$	(111)	Ag	0	2.49	1.85
$CH_4^* \rightarrow CH_3^* + H^*$	(111)	Au	0	2.23	1.58
$CH_4^* \rightarrow CH_3^* + H^*$	(111)	Rh	0	1.08	0.51

TS12 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$CH_4^* \rightarrow CH_3^* + H^*$	(211)	Pt	0	0.73	-0.06
$CH_4^* \rightarrow CH_3^* + H^*$	(211)	Pd	0	0.83	0.35
$CH_4^* \rightarrow CH_3^* + H^*$	(211)	Ru	0	0.52	-0.55
$CH_4^* \rightarrow CH_3^* + H^*$	(211)	Re	0	0.49	-0.92
$CH_4^* \rightarrow CH_3^* + H^*$	(211)	Co	0	0.86	-0.75
$CH_4^* \rightarrow CH_3^* + H^*$	(211)	Ni	0	1.13	-0.12
$CH_4^* \rightarrow CH_3^* + H^*$	(211)	Mn	0	0.68	-0.66
$CH_4^* \rightarrow CH_3^* + H^*$	(211)	Cu	0	1.7	0.89
$CH_4^* \rightarrow CH_3^* + H^*$	(211)	Ag	0	2.23	1.65
$CH_4^* \rightarrow CH_3^* + H^*$	(211)	Au	0	1.83	1.2
$CH_4^* \rightarrow CH_3^* + H^*$	(211)	Rh	0	0.66	-0.16

TS13 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*

$CH_3^* \rightarrow CH_2^* + H^*$	(111)	Pt	0.55	1.53	0.84
$CH_3^* \rightarrow CH_2^* + H^*$	(111)	Pd	0.92	1.95	1.27
$CH_3^* \rightarrow CH_2^* + H^*$	(111)	Ru	0.73	1.43	0.76
$CH_3^* \rightarrow CH_2^* + H^*$	(111)	Re	0.5	1.24	0.14
$CH_3^* \rightarrow CH_2^* + H^*$	(111)	Co	0.89	1.65	1.1
$CH_3^* \rightarrow CH_2^* + H^*$	(111)	Ni	0.93	1.73	1.06
$CH_3^* \rightarrow CH_2^* + H^*$	(111)	Mn	0.15	0.89	-0.03
$CH_3^* \rightarrow CH_2^* + H^*$	(111)	Cu	1.3	2.87	2.28
$CH_3^* \rightarrow CH_2^* + H^*$	(111)	Ag	1.6	3.99	3.29
$CH_3^* \rightarrow CH_2^* + H^*$	(111)	Au	1.35	3.45	2.87
$CH_3^* \rightarrow CH_2^* + H^*$	(111)	Rh	0.84	1.44	1.01

TS14 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$CH_3^* \rightarrow CH_2^* + H^*$	(211)	Pt	0.46	0.94	0.25
$CH_3^* \rightarrow CH_2^* + H^*$	(211)	Pd	0.79	1.53	0.84
$CH_3^* \rightarrow CH_2^* + H^*$	(211)	Ru	0.06	0.68	0.08
$CH_3^* \rightarrow CH_2^* + H^*$	(211)	Re	-0.13	0.28	-0.58
$CH_3^* \rightarrow CH_2^* + H^*$	(211)	Co	0.04	0.99	0.01
$CH_3^* \rightarrow CH_2^* + H^*$	(211)	Ni	0.39	1.41	0.63
$CH_3^* \rightarrow CH_2^* + H^*$	(211)	Mn	0.02	0.69	-0.19
$CH_3^* \rightarrow CH_2^* +$	(211)	Cu	0.97	2.5	2.15

H^*					
$CH_3^* \rightarrow CH_2^* + H^*$	(211)	Ag	1.39	3.52	3.14
$CH_3^* \rightarrow CH_2^* + H^*$	(211)	Au	1.1	2.81	2.34
$CH_3^* \rightarrow CH_2^* + H^*$	(211)	Rh	0.36	0.79	0.25

TS15 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$CH_2^* \rightarrow CH^* + H^*$	(111)	Pt	1.21	1.8	0.86
$CH_2^* \rightarrow CH^* + H^*$	(111)	Pd	1.64	2.24	1.38
$CH_2^* \rightarrow CH^* + H^*$	(111)	Ru	1.17	1.39	0.72
$CH_2^* \rightarrow CH^* + H^*$	(111)	Re	0.64	0.84	0.08
$CH_2^* \rightarrow CH^* + H^*$	(111)	Co	1.45	1.73	1.16
$CH_2^* \rightarrow CH^* + H^*$	(111)	Ni	1.44	1.78	1.1
$CH_2^* \rightarrow CH^* + H^*$	(111)	Mn	0.65	0.97	0.23
$CH_2^* \rightarrow CH^* + H^*$	(111)	Cu	2.35	3.52	2.77
$CH_2^* \rightarrow CH^* + H^*$	(111)	Ag	3.04	4.9	4.22
$CH_2^* \rightarrow CH^* + H^*$	(111)	Au	2.65	4.26	3.45
$CH_2^* \rightarrow CH^* + H^*$	(111)	Rh	1.33	1.4	0.88

TS16 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$CH_2^* \rightarrow CH^* + H^*$	(211)	Pt	0.76	2.35	0.67
$CH_2^* \rightarrow CH^* + H^*$	(211)	Pd	1.28	2.05	1.13
$CH_2^* \rightarrow CH^* + H^*$	(211)	Ru	0.69	1.07	0.1

$CH_2^* \rightarrow CH^* + H^*$	(211)	Re	0.21	0.6	-0.73
$CH_2^* \rightarrow CH^* + H^*$	(211)	Co	0.79	1.78	0.38
$CH_2^* \rightarrow CH^* + H^*$	(211)	Ni	1.14	1.93	0.63
$CH_2^* \rightarrow CH^* + H^*$	(211)	Mn	0.49	0.64	-0.32
$CH_2^* \rightarrow CH^* + H^*$	(211)	Cu	2.22	3.27	2.63
$CH_2^* \rightarrow CH^* + H^*$	(211)	Ag	2.87	4.74	4.18
$CH_2^* \rightarrow CH^* + H^*$	(211)	Au	2.23	4.58	3.53
$CH_2^* \rightarrow CH^* + H^*$	(211)	Rh	0.76	1.54	0.49

TS17 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$CH^* \rightarrow C^* + H^*$	(111)	Pt	1.23	3.1	1.9
$CH^* \rightarrow C^* + H^*$	(111)	Pd	1.74	3.12	2.16
$CH^* \rightarrow C^* + H^*$	(111)	Ru	1.14	2.53	1.62
$CH^* \rightarrow C^* + H^*$	(111)	Re	0.57	1.96	0.98
$CH^* \rightarrow C^* + H^*$	(111)	Co	1.51	2.81	2.06
$CH^* \rightarrow C^* + H^*$	(111)	Ni	1.48	2.87	2.07
$CH^* \rightarrow C^* + H^*$	(111)	Mn	0.91	1.81	0.96
$CH^* \rightarrow C^* + H^*$	(111)	Cu	2.85	5.06	4.34
$CH^* \rightarrow C^* + H^*$	(111)	Ag	3.96	6.53	5.91
$CH^* \rightarrow C^* + H^*$	(111)	Au	3.23	5.81	5
$CH^* \rightarrow C^* + H^*$	(111)	Rh	1.21	2.56	1.64

TS18 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$CH^* \rightarrow C^* + H^*$	(211)	Pt	1.19	3.06	1.58
$CH^* \rightarrow C^* + H^*$	(211)	Pd	1.57	2.25	1.14
$CH^* \rightarrow C^* + H^*$	(211)	Ru	0.71	1.74	0.58

$CH^* \rightarrow C^* + H^*$	(211)	Re	0.06	1.28	-0.5
$CH^* \rightarrow C^* + H^*$	(211)	Co	1.16	2.18	0.61
$CH^* \rightarrow C^* + H^*$	(211)	Mn	0.36	1.32	-0.06
$CH^* \rightarrow C^* + H^*$	(211)	Cu	2.7	4.31	3.49
$CH^* \rightarrow C^* + H^*$	(211)	Ag	3.92	5.99	5.32
$CH^* \rightarrow C^* + H^*$	(211)	Au	3.43	5.78	4.86
$CH^* \rightarrow C^* + H^*$	(211)	Rh	1.01	1.97	1.08

TS19 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$C_2H_6^* (g) \rightarrow C_2H_5^* + H^*$	(211)	Ag	0.79598	3.0385878	2.559831
$C_2H_6^* (g) \rightarrow C_2H_5^* + H^*$	(211)	Au	0.79598	2.5852867	2.041831
$C_2H_6^* (g) \rightarrow C_2H_5^* + H^*$	(211)	Cu	0.79598	2.5205934	1.835831
$C_2H_6^* (g) \rightarrow C_2H_5^* + H^*$	(211)	Pt	0.79598	1.4777445	0.701831
$C_2H_6^* (g) \rightarrow C_2H_5^* + H^*$	(211)	Rh	0.79598	1.4768537	0.737831

TS20 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$C_2H_4^* \rightarrow C_2H_3^* + H^*$	(211)	Ag	2.393662	4.9239478	3.741662
$C_2H_4^* \rightarrow C_2H_3^* + H^*$	(211)	Au	2.393662	4.9001974	3.403662
$C_2H_4^* \rightarrow C_2H_3^* + H^*$	(211)	Cu	2.263662	4.1803106	2.937662
$C_2H_4^* \rightarrow C_2H_3^* + H^*$	(211)	Pt	1.583662	3.1637368	1.443662
$C_2H_4^* \rightarrow C_2H_3^* + H^*$	(211)	Rh	1.483662	2.5702706	1.349662

TS21 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$C_2H_5^* \rightarrow C_2H_4^* + H^*$	(211)	Ag	2.2977465	3.3983752	2.6557465
$C_2H_5^* \rightarrow C_2H_4^* + H^*$	(211)	Au	1.9377465	3.3684785	2.4977465
$C_2H_5^* \rightarrow C_2H_4^* + H^*$	(211)	Cu	1.9077465	2.794904	2.1917465
$C_2H_5^* \rightarrow C_2H_4^* + H^*$	(211)	Pt	1.2177465	1.987584	1.0677465
$C_2H_5^* \rightarrow C_2H_4^* + H^*$	(211)	Rh	1.2577465	1.6106883	0.9637465

TS22 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$C_3H_8^* \rightarrow C_3H_7^* + H^*$	(211)	Ag	1.556975	3.8278035	3.265444
$C_3H_8^* \rightarrow C_3H_7^* + H^*$	(211)	Au	1.556975	3.6463738	2.767673
$C_3H_8^* \rightarrow C_3H_7^* + H^*$	(211)	Cu	1.556975	3.5744228	2.545687

$C_3H_8^* \rightarrow C_3H_7^* + H^*$	(211)	Pt	1.556975	2.548565	1.481978
$C_3H_8^* \rightarrow C_3H_7^* + H^*$	(211)	Rh	1.556975	2.560761	1.498891
$C_3H_8^* \rightarrow C_3H_7^* + H^*$	(211)	Ru	1.556975	2.3494497	1.096529

TS23 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$C_3H_6^* \rightarrow C_3H_5^* + H^*$	(211)	Ag	1.556975	3.8278035	3.265444
$C_3H_6^* \rightarrow C_3H_5^* + H^*$	(211)	Au	1.556975	3.6463738	2.767673
$C_3H_6^* \rightarrow C_3H_5^* + H^*$	(211)	Cu	1.556975	3.5744228	2.545687
$C_3H_6^* \rightarrow C_3H_5^* + H^*$	(211)	Pt	1.556975	2.548565	1.481978
$C_3H_6^* \rightarrow C_3H_5^* + H^*$	(211)	Rh	1.556975	2.560761	1.498891
$C_3H_6^* \rightarrow C_3H_5^* + H^*$	(211)	Ru	1.556975	2.3494497	1.096529

TS24 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
$CH_4^* \rightarrow CH_3^* + H^*$	(0001)	Co	0	1.2379743	0.200979
$CH_3^* \rightarrow CH_2^* + H^*$	(0001)	Co	0.6050025	1.370704	0.9488455
$CH_2^* \rightarrow CH^* + H^*$	(0001)	Co	1.352869	1.789418	0.966225
$CH^* \rightarrow C^* + H^*$	(0001)	Co	1.3702485	2.1680427	1.3937755
$CH_3CH_3^* \rightarrow CH_2CH_3^* + H^*$	(0001)	Co	0.79598	2.1859693	1.108219
$CH_3CH_2CH_3^* \rightarrow CH_2CH_2CH_3^* + H^*$	(0001)	Co	1.556975	2.9648222	1.841591
$CH_2CH_2^* \rightarrow CHCH_2^* +$	(0001)	Co	2.411861	3.2828193	2.463037

H^*					
$CH_2CHCH_3^*$ -> $CHCH_2CH_3^* + H^*$	(0001)	Co	2.999589	4.2004175	3.269306

TS25 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
H_2^* -> $2H^*$	(111)	Pd	0	0,12	-0,73
H_2^* -> $2H^*$	(111)	Pt	0	0,19	-0,67
H_2^* -> $2H^*$	(0001)	Ru	0	1,23	0,95
H_2^* -> $2H^*$	(111)	Au	0	1,15	0,58
H_2^* -> $2H^*$	(111)	Cu	0	0,78	-0,08
H_2^* -> $2H^*$	(100)	Pt	0	0,11	-0,91

TS26 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
H_2^* -> $2H^*$	(211)	Pt	0	0,09	-0,98
H_2^* -> $2H^*$	(211)	Cu	0	0,68	0,24
H_2^* -> $2H^*$	(211)	Au	0	0,98	0,31
H_2^* -> $2H^*$	(211)	Ag	0	0,99	0,63
H_2^* -> $2H^*$	(211)	Pd	0	0,55	0,29

TS27 The studied reaction, structural information and relevant energies.

Reaction	*Surface*	*Metal*	*Initial state energy [eV]*	*Transition state energy [eV]*	*Final state energy [eV]*
OOH^* -> $O_2^* + H^*$	M12	Au	4.06	5.46	4.79

$H_2O_2^* \rightarrow OOH^* + H^*$	M12	Au	3.30	4.45	3.98

TS28 The studied reaction, structural information and relevant energies.