

Supporting Information

for

A Prediction Model for CO₂/CO Adsorption Performance on Binary Alloys Based on Machine Learning

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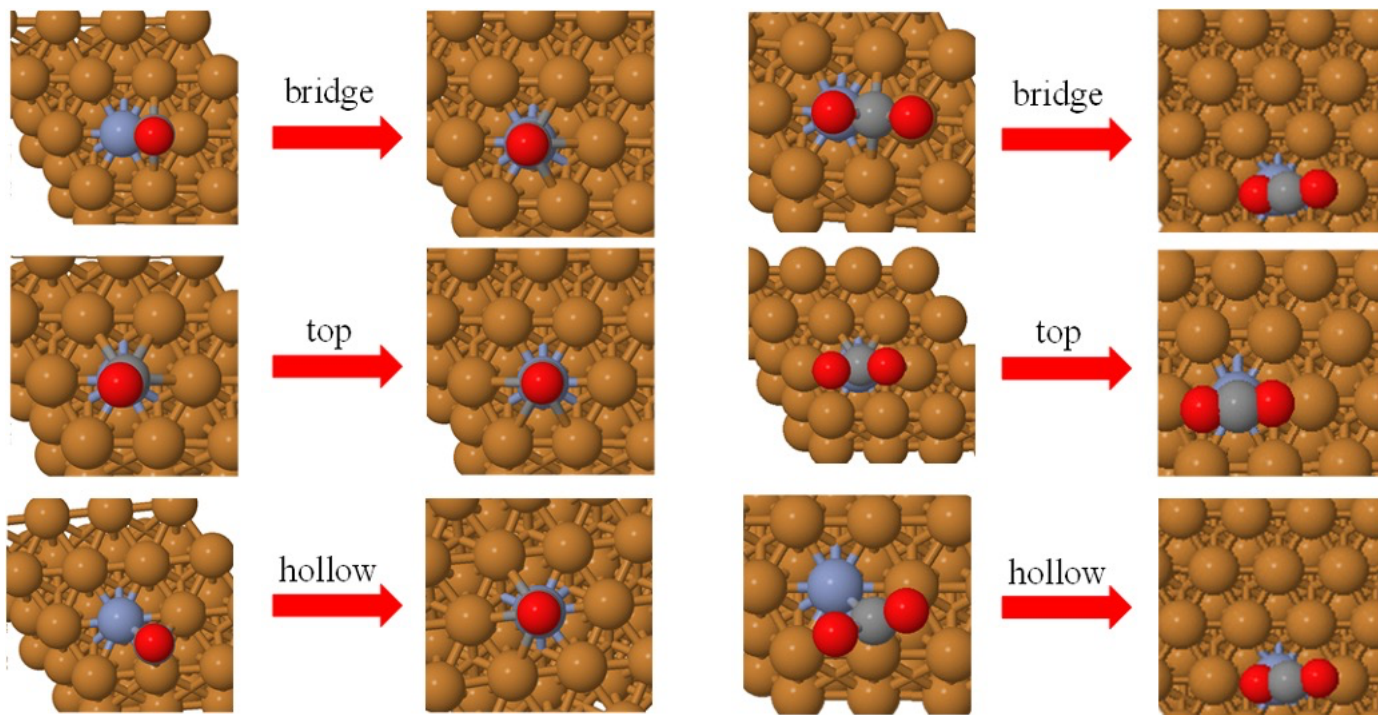


Figure S1 Processes of geometric optimization show that both CO (left) and CO₂ (right) relax to the top sites no matter which site the adsorbates are initially positioned on.

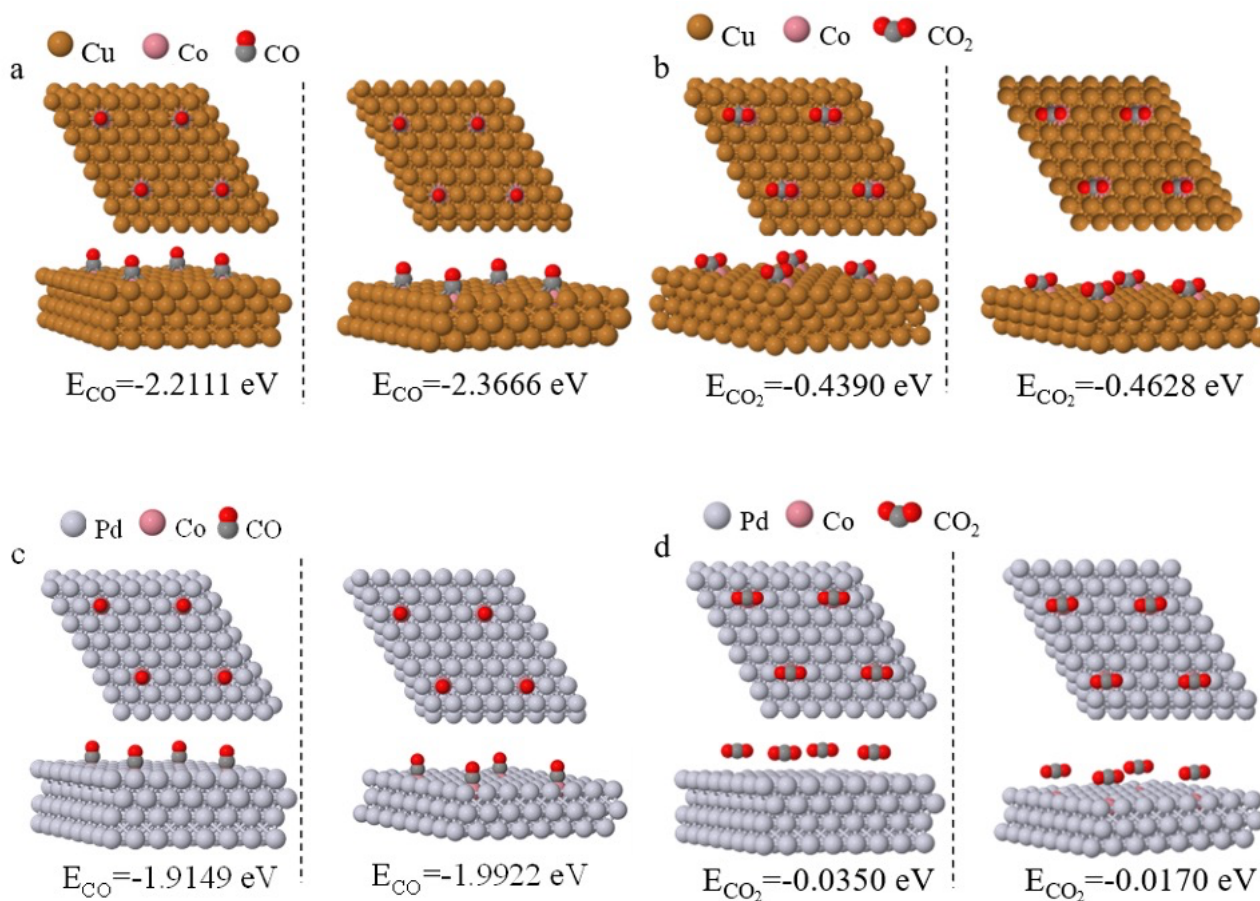


Figure S2 Comparison of adsorption energy between three-layer and four-layer units. (a) and (b) Comparison of CO/CO₂ adsorption energies of Cu/Co three- and four-layer; (c) and (d) Comparison of CO/CO₂ adsorption energies of Pd/Co three- and four-layer.

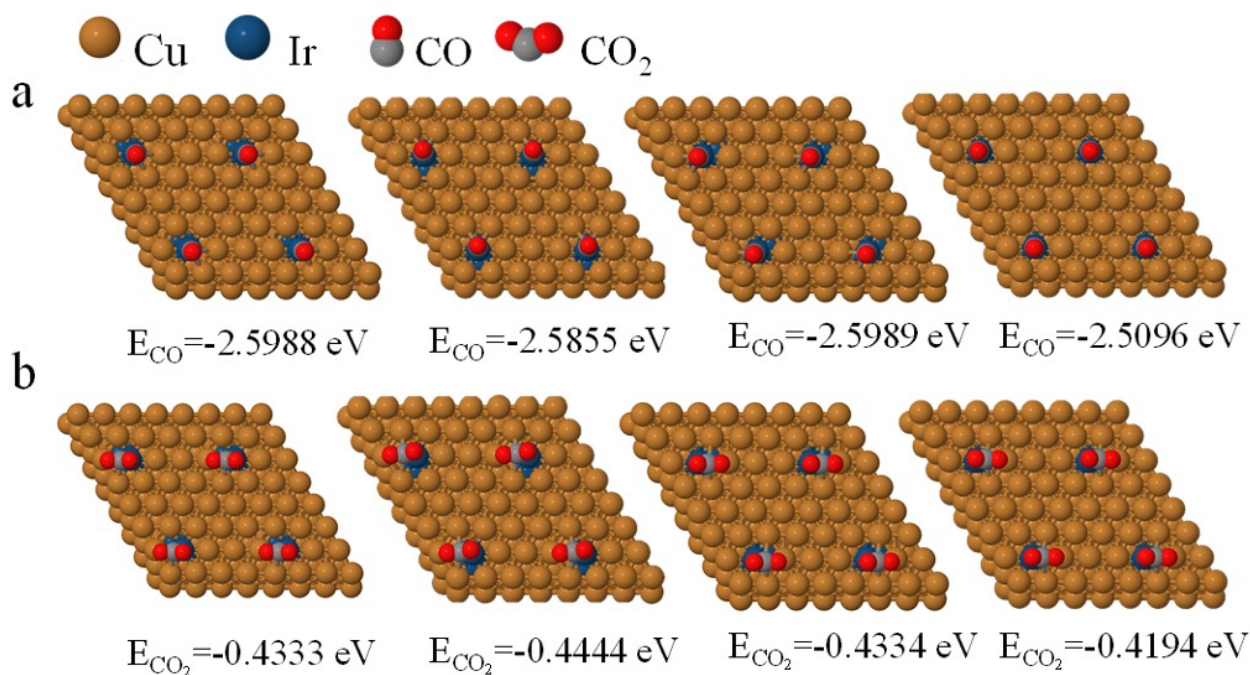


Figure S3. Effect of double-atom doping compared with single-atom doping on E_{ads} of (a) CO and (b) CO₂. The alloy is Ir/Cu and first three figures on each row are double-atom doping, while the rightmost figure is single-atom doping.

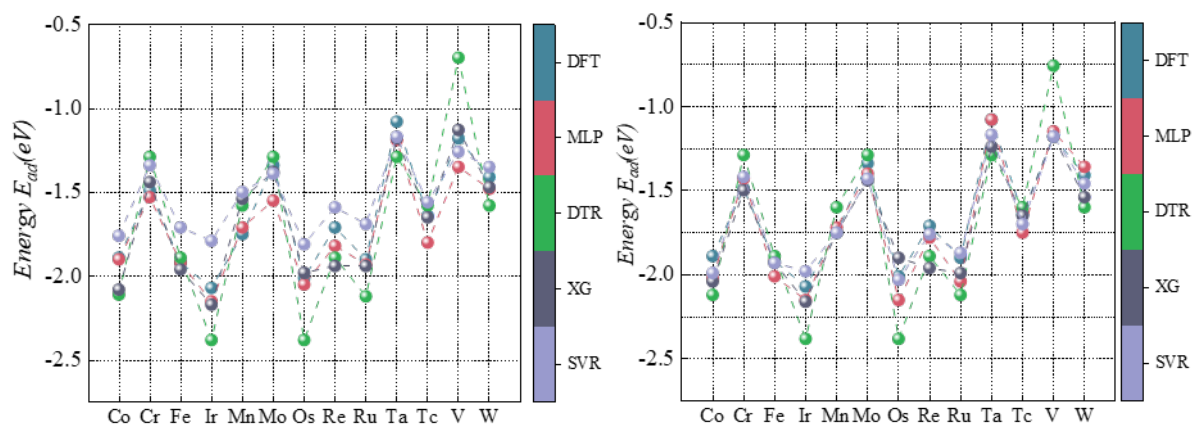


Figure S4 Comparison of CO E_{ads} between four ML predictions and DFT ML models and DFT: Prediction 1 (left); Prediction 2 (right).

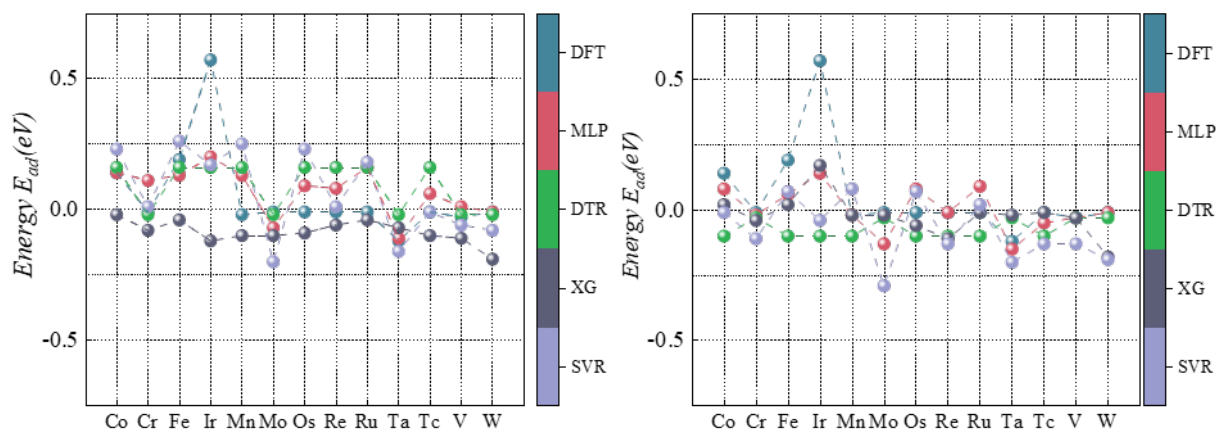


Figure S5 Comparison of CO₂ E_{ads} between four ML predictions and DFT: Prediction 1 (left); Prediction 2 (right)

Table S1 List of 74 features associated with each alloy material used in the ML model of this study

Code Name of Features	Meaning of Features	ID
E_O	Adsorption energy of O by M1/M2	1
E_H	Adsorption energy of H by M1/M2	2
R_1	Radius of M1	3
R_2	Radius of M2	4
R_differ	$R_1 - R_2$	5
R_sum	$R_1 + R_2$	6
R_product	$R_1 \times R_2$	7
R_division	$R_1 \div R_2$	8
AE_1	First electron affinity of M1	9
AE_2	First electron affinity of M2	10
AE_differ	$AE_1 - AE_2$	11
AE_sum	$AE_1 + AE_2$	12
AE_product	$AE_1 \times AE_2$	13
AE_division	$AE_1 \div AE_2$	14
g_1	Density of M1	15
g_2	Density of M2	16
g_differ	$g_1 - g_2$	17
g_sum	$g_1 + g_2$	18
g_product	$g_1 \times g_2$	19
g_division	$g_1 \div g_2$	20
H_1	Standard molar enthalpy of formation of M1	21
H_2	Standard molar enthalpy of formation of M2	22
H_differ	$H_1 - H_2$	23
H_sum	$H_1 + H_2$	24
H_product	$H_1 \times H_2$	25
H_division	$H_1 \div H_2$	26
C_1	Specific heat capacity of M1	27
C_2	Specific heat capacity of M2	28
C_differ	$C_1 - C_2$	29
C_sum	$C_1 + C_2$	30
C_product	$C_1 \times C_2$	31
C_division	$C_1 \div C_2$	32
G_1	Standard molar Gibbs free energy of formation of M1	33
G_2	Standard molar Gibbs free energy of formation of M2	34
G_differ	$G_1 - G_2$	35
G_sum	$G_1 + G_2$	36
G_product	$G_1 \times G_2$	37
G_division	$G_1 \div G_2$	38
S_1	Standard molar entropy of M1	39
S_2	Standard molar entropy of M2	40
S_differ	$S_1 - S_2$	41
S_sum	$S_1 + S_2$	42
S_product	$S_1 \times S_2$	43

Code Name of Features	Meaning of Features	ID
S_division	$S_1 \div S_2$	44
AN_1	Atomic number of M1	45
AN_2	Atomic number of M2	46
AN_differ	$AN_1 - AN_2$	47
AN_sum	$AN_1 + AN_2$	48
AN_product	$AN_1 \times AN_2$	49
AN_division	$AN_1 \div AN_2$	50
PN_1	Period of the element of M1	51
PN_2	Period of the element of M2	52
PN_differ	$PN_1 - PN_2$	53
PN_sum	$PN_1 + PN_2$	54
PN_product	$PN_1 \times PN_2$	55
PN_division	$PN_1 \div PN_2$	56
GN_1	IUPAC group number of M1	57
GN_2	IUPAC group number of M2	58
GN_differ	$GN_1 - GN_2$	59
GN_sum	$GN_1 + GN_2$	60
GN_product	$GN_1 \times GN_2$	61
GN_division	$GN_1 \div GN_2$	62
EN_1	Electronegativity of M1	63
EN_2	Electronegativity of M2	64
EN_differ	$EN_1 - EN_2$	65
EN_sum	$EN_1 + EN_2$	66
EN_product	$EN_1 \times EN_2$	67
EN_division	$EN_1 \div EN_2$	68
FE_1	First ionization energy of M1	69
FE_2	First ionization energy of M2	70
FE_differ	$FE_1 - FE_2$	71
FE_sum	$FE_1 + FE_2$	72
FE_product	$FE_1 \times FE_2$	73
FE_division	$FE_1 \div FE_2$	74

Table S2 DFT calculation results

Name	E_O (eV)	E_H (eV)	E_CO ₂ (eV)	E_CO (eV)
Ag_Co	0.420556	-0.29126	-0.2154	-2.33778
Ag_Cr	-1.29417	-0.06932	-0.55266	-2.20352
Ag_Fe	-0.09741	-0.32693	-0.4661	-2.58491
Ag_Ir	1.097783	-0.70461	0.0603	-2.55684
Ag_Mn	-0.69349	-0.27392	-0.6392	-2.59237
Ag_Mo	-1.42292	-0.29354	-0.7882	-2.56587
Ag_Os	-0.16917	-0.81183	-0.4401	-3.0549
Ag_Re	-1.27865	-0.71325	-0.7397	-3.08243
Ag_Ru	0.401478	-0.49323	-0.3515	-2.69537
Ag-Ta	-2.14492	-0.30886	-1.082	-2.15923
Ag_Tc	-0.80362	-0.45615	-0.6179	-2.81404
Ag_V	-1.59849	-0.06047	-0.8351	-2.00839
Ag_W	-2.04263	-0.50969	-1.0117	-2.77271
Au_Co	1.265792	-0.07887	0.3733	-1.97175
Au_Cr	-0.47431	-1.83212	0.105581	0.29772
Au_Fe	0.73728	-0.1428	0.2343	-2.17984
Au_Ir	1.52641	-2.19685	-0.4635	0.699409
Au_Mn	0.061009	-0.10269	0.1467	-2.17424
Au_Mo	-0.65965	-1.94005	0.000908	0.307236
Au_Os	0.428914	-2.55049	-0.55709	0.379894
Au_Re	-0.52798	-2.41719	-0.46199	0.310027
Au_Ru	0.922749	-0.38067	0.247	-2.36111
Au-Ta	-1.07215	-1.54017	0.211358	0.277347
Au_Tc	-0.19715	-0.3443	0.1288	-2.3868
Au_V	-0.84224	0.213106	0.122	-1.64636
Au_W	-1.17238	-2.09188	-0.19484	0.212967
Cu_Co	-0.14784	-0.21505	-0.4628	-2.3666
Cu_Cr	-1.16078	-0.06876	-0.865	-2.21112
Cu_Fe	-0.51006	-0.2156	-0.6722	-2.54118
Cu_Ir	0.407833	-0.58578	-0.2194	-2.5097
Cu_Mn	-0.64865	-0.15586	-0.7911	-2.47534
Cu_Mo	-1.25155	-0.73485	-0.7996	-2.23833
Cu_Os	-0.13151	-0.60824	-0.5394	-2.86272
Cu_Re	-1.15528	-0.50853	-0.7315	-2.78193
Cu_Ru	0.388724	-0.30908	-0.5058	-2.54854
Cu-Ta	-1.77647	-0.2489	-1.1292	-1.86769
Cu_Tc	-0.74554	-0.25052	-0.6805	-2.54647
Cu_V	-1.40356	0.027146	-0.9254	-1.81855
Cu_W	-1.78465	-0.39129	-0.9721	-2.43821
Ni_Co	1.216609	-0.20635	-0.07	-2.15709
Ni_Cr	-0.14151	0.163051	-0.4421	-1.61682
Ni_Fe	0.669756	-0.17171	-0.1871	-2.15909

Name	E_O (eV)	E_H (eV)	E_CO ₂ (eV)	E_CO (eV)
Ni_Ir	1.289543	-0.51973	-0.0135	-2.2669
Ni_Mn	0.163913	-0.05726	-0.1664	-1.94133
Ni_Mo	-0.23976	0.251494	-0.1165	-1.42178
Ni_Os	0.331197	-0.39497	0.0136	-2.17313
Ni_Re	-0.31458	-0.15948	-0.305	-1.80423
Ni_Ru	0.753134	-0.20116	-0.0658	-2.10421
Ni-Ta	-0.25836	0.393254	-0.2104	-1.14839
Ni_Tc	-0.05907	-0.01444	-0.0477	-1.77172
Ni_V	-0.11816	0.48666	-0.0934	-1.26572
Ni_W	-0.57346	0.123517	-0.0745	-1.48302
Pt_Co	0.630747	0.005265	0.05501	-1.85752
Pt_Cr	0.113354	0.241697	0.20854	-1.4189
Pt_Fe	0.989116	-0.0413	0.157075	-1.87653
Pt_Ir	1.464066	-0.47454	0.155515	-2.24906
Pt_Mn	0.466366	0.058381	0.134021	-1.70884
Pt_Mo	-0.03901	0.370604	-0.00904	-1.27187
Pt_Os	0.4837	-0.37729	0.077576	-2.10756
Pt_Re	-0.16	-0.12962	0.175927	-1.63897
Pt_Ru	0.938547	-0.14679	0.164007	-2.02198
Pt-Ta	0.167152	0.738235	-0.07953	-0.98884
Pt_Tc	0.085934	0.031458	0.064424	-1.63945
Pt_V	0.180359	0.672037	0.119439	-1.13002
Pt_W	-0.31887	0.288158	0.031656	-1.32266
Co_Co	0.022756	0.404726	0.174453	-1.4233
Co_Cr	0.349613	0.201027	-0.15438	-1.67442
Co_Fe	1.407772	0.012469	0.075265	-1.83575
Co_Ir	2.799158	0.495524	0.208555	-0.68253
Co_Mn	3.201122	0.964892	0.210821	-0.00985
Co_Mo	0.445731	0.796056	-0.17653	-0.74417
Co_Os	-0.0944	0.447167	0.070343	-1.27517
Co_Re	1.904573	-0.03029	0.210299	-1.69368
Co_Ru	3.774922	0.757693	0.222683	-0.2341
Co-Ta	0.57956	0.720482	-0.21528	-0.8067
Co_Tc	-0.25327	0.432499	-0.03072	-1.08013
Co_V	-0.1586	0.070998	0.255478	-1.63852
Co_W	0.551225	-0.12565	0.211724	-1.83119

Table S3 Optimal combination of features for predicting E_{ads} of CO found in each step of the greedy algorithm

Optimal combination of features found in this step	Step number	RMSE (eV)
[2]	2	0.65205
[2, 63]	136	0.40355
[2, 63, 27]	173	0.35834
[2, 63, 27, 62]	279	0.33368
[2, 63, 27, 62, 69]	355	0.29882
[2, 63, 27, 62, 69, 1]	361	0.28046
[2, 63, 27, 62, 69, 1, 45]	471	0.27099
[2, 63, 27, 62, 69, 1, 45, 9]	504	0.26643
[2, 63, 27, 62, 69, 1, 45, 9, 57]	616	0.26102
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26]	653	0.25774
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21]	713	0.25353
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61]	812	0.24997
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3]	823	0.24532
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31]	908	0.2423
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72]	1003	0.23979
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33]	1030	0.23742
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15]	1075	0.23572
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59]	1169	0.23422
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39]	1243*	0.2337
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30]	1257	0.23403
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43]	1321	0.23468
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60]	1388	0.23573
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35]	1421	0.23696
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12]	1457	0.23763
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19]	1513	0.2381
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58]	1590	0.23914
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32]	1619	0.24069
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18]	1659	0.24262
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44]	1720	0.24431
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 20]	1752	0.24701
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 20, 7]	1797	0.24864
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 20, 7, 37]	1833	0.25179
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 20, 7, 37, 6]	1891	0.25451
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 20, 7, 37, 6, 8]	1917	0.25633
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 20, 7, 37, 6, 8, 48]	1958	0.25834
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 20, 7, 37, 6, 8, 48, 36]	2017	0.26063
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 20, 7, 37, 6, 8, 48, 36, 23]	2050	0.2631
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 20, 7, 37, 6, 8, 48, 36, 23, 50]	2082	0.26632
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 20, 7, 37, 6, 8, 48, 36, 23, 50]	2130	0.26982

Optimal combination of features found in this step	Step number	RMSE (eV)
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25]	2156	0.27411
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11]	2184	0.27835
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41]	2229	0.2825
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49]	2264	0.28677
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73]	2309	0.2914
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74]	2340	0.29541
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56]	2362	0.29971
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38]	2382	0.30393
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24]	2406	0.30796
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4]	2425	0.31197
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71]	2475	0.31683
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16]	2480	0.32168
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5]	2500	0.32722
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55]	2538	0.3326
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54]	2559	0.33785
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51]	2577	0.34368
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70]	2604	0.34967
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34]	2612	0.3561
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29]	2629	0.36246
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22]	2644	0.36955
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46]	2662	0.37661
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52]	2678	0.3832

Optimal combination of features found in this step	Step number	RMSE (eV)
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10]	2685	0.38968
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28]	2701	0.39487
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47]	2714	0.40103
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47, 17]	2723	0.4061
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47, 17, 53]	2734	0.41102
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47, 17, 53, 66]	2745	0.41826
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47, 17, 53, 66, 40]	2750	0.42506
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47, 17, 53, 66, 40, 14]	2756	0.43113
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47, 17, 53, 66, 40, 14, 67]	2764	0.43677
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47, 17, 53, 66, 40, 14, 67, 13]	2766	0.44325
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47, 17, 53, 66, 40, 14, 67, 68, 13, 65]	2774	0.45851
[2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47, 17, 53, 66, 40, 14, 67, 68, 13, 65, 64]	2775	0.46775

* Features of the lowest RMSE optimized by greedy algorithm

Table S4 Optimal combination of features for predicting E_{ads} of CO_2 found in each step of the greedy algorithm

Optimal combination of features found in this step	Step number	RMSE (eV)
[1]	1	0.27957
[1, 69]	142	0.22727
[1, 69, 57]	203	0.19097
[1, 69, 57, 2]	220	0.16572
[1, 69, 57, 2, 63]	350	0.15109
[1, 69, 57, 2, 63, 58]	415	0.14759
[1, 69, 57, 2, 63, 58, 61]	486	0.13944
[1, 69, 57, 2, 63, 58, 61, 6]	501	0.13963
[1, 69, 57, 2, 63, 58, 61, 6, 60]	619	0.13352
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37]	664	0.13085
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27]	719	0.12372
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59]	811	0.12266
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62]	874	0.11824
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45]	924	0.12258
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36]	977	0.1169
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26]	1028	0.11674
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34]	1093	0.11536
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38]	1152	0.11391
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35]	1208	0.1147
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3]	1243*	0.11259
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23]	1309	0.1173
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24]	1363	0.11474
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22]	1415	0.11408
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9]	1454	0.1228
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21]	1516	0.116
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33]	1572	0.11204
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18]	1612	0.11173
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19]	1660	0.11203
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49]	1723	0.11372
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55]	1774	0.11182
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48]	1813	0.1141
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8]	1833	0.12334
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4]	1873	0.128
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7]	1916	0.12081
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5]	1956	0.12876
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15]	2001	0.11545
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54]	2061	0.11645
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16]	2078	0.11555
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31]	2121	0.11537

Optimal combination of features found in this step	Step number	RMSE (eV)
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30]	2156	0.11552
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32]	2191	0.11535
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50]	2233	0.11671
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17]	2253	0.11617
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25]	2286	0.11608
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20]	2316	0.11681
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52]	2357	0.11838
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51]	2385	0.1187
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47]	2412	0.11899
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56]	2440	0.12001
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53]	2465	0.12045
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46]	2489	0.12116
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74]	2522	0.12059
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72]	2543	0.13031
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73]	2565	0.12167
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71]	2585	0.12227
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28]	2591	0.1226
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29]	2610	0.12515
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70]	2639	0.13357
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41]	2647	0.12958
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42]	2663	0.13122
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43]	2678	0.13329

Optimal combination of features found in this step	Step number	RMSE (eV)
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44]	2692	0.13489
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39]	2703	0.13786
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39, 11]	2711	0.14113
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39, 11, 12]	2722	0.1435
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39, 11, 12, 14]	2733	0.149
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39, 11, 12, 14, 68]	2747	0.15202
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39, 11, 12, 14, 68, 65]	2752	0.15498
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39, 11, 12, 14, 68, 65, 66]	2759	0.15864
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39, 11, 12, 14, 68, 65, 66, 67]	2765	0.16204
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39, 11, 12, 14, 68, 65, 66, 67, 40]	2768	0.16519
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39, 11, 12, 14, 68, 65, 66, 67, 40, 13]	2771	0.16892
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39, 11, 12, 14, 68, 65, 66, 67, 40, 13, 10]	2773	0.17373
[1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39, 11, 12, 14, 68, 65, 66, 67, 40, 13, 10, 64]	2775	0.1791

* Features of the lowest RMSE optimized by greedy algorithm

Table S5. Results of four machine learning algorithms for predicting CO₂ adsorption energy on Rh surfaces

Parameters and results	Co	Cr	Fe	Ir	Mn	Mo	Os	Re	Ru	Ta	Tc	V	W	MAE (eV)
DFT	0.14	-0.01	0.19	0.57	-0.02	-0.01	-0.01	-0.01	-0.01	-0.12	-0.01	-0.03	-0.01	
M Prediction 1/eV	0.14	0.11	0.13	0.20	0.13	-0.07	0.09	0.08	0.16	-0.11	0.06	0.01	-0.01	0.10
L Error (eV)**	0.00	0.12	0.06	0.37	-0.15	0.06	-0.10	-0.09	-0.17	-0.01	-0.07	-0.04	0.00	
P Prediction 2/eV	0.08	-0.02	0.06	0.14	-0.02	-0.13	0.08	-0.01	0.09	-0.15	-0.05	-0.03	-0.01	0.08
P Error (eV)**	0.06	0.01	0.13	0.43	0.00*	0.12	-0.09	0.00	-0.10	0.03	0.04	0.00*	0.00	
D Prediction 1/eV	0.16	-0.02	0.16	0.16	0.16	-0.02	0.16	0.16	0.16	-0.02	0.16	-0.02	-0.02	0.11
T Error (eV)**	-0.02	0.01	0.03	0.41	-0.18	0.01	-0.17	-0.17	-0.17	-0.10	-0.17	0.01	0.01	
R Prediction 2/eV	-0.10	-0.03	-0.10	-0.10	-0.10	-0.03	-0.10	-0.10	-0.10	-0.03	-0.10	-0.03	-0.03	0.14
R Error (eV)**	0.24	0.02	0.29	0.67	0.08*	0.02	0.09	0.09	0.09	-0.09	0.09	0.00*	0.02	
Prediction 1/eV	-0.02	-0.08	-0.04	-0.12	-0.10	-0.10	-0.09	-0.06	-0.04	-0.07	-0.10	-0.11	-0.19	0.13
X Error (eV)**	0.16	0.07	0.23	0.45	0.08	0.09	0.08	0.05	0.03	-0.05	0.09	0.08	0.18	
G Prediction 2/eV	0.02	-0.04	0.02	0.17	-0.02	-0.02	-0.06	-0.11	-0.01	-0.02	-0.01	-0.03	-0.18	0.09
G Error (eV)**	0.12	0.03	0.17	0.40	0.00*	0.01	0.05	0.10	0.00	-0.10	0.00	0.00*	0.17	
S Prediction 1/eV	0.23	0.01	0.26	0.17	0.25	-0.20	0.23	0.01	0.18	-0.16	-0.01	-0.06	-0.08	0.13
V Error (eV)**	-0.09	-0.02	0.07	0.40	-0.27	0.19	-0.24	-0.02	-0.19	0.04	0.00	0.03	0.07	
R Prediction 2/eV	-0.01	-0.11	0.07	-0.04	0.08	-0.29	0.07	-0.13	0.02	-0.20	-0.13	-0.13	-0.19	0.16
R Error (eV)**	0.15	0.10	0.12	0.61	-0.10*	0.28	-0.08	0.12	-0.03	0.08	0.12	0.10*	0.18	

* These cases are part of the training set; therefore, small errors are expected.

** Error between DFT and predicted value

Table S6. Results of four machine learning algorithms for predicting CO adsorption energy on Rh surfaces

Parameters and results	Co	Cr	Fe	Ir	Mn	Mo	Os	Re	Ru	Ta	Tc	V	W	MAE (eV)
DFT/eV	-1.89	-1.49	-1.92	-2.07	-1.75	-1.34	-2.01	-1.71	-1.90	-1.08	-1.64	-1.18	-1.41	
M prediction 1/eV	-1.90	-1.53	-1.92	-2.15	-1.71	-1.55	-2.05	-1.82	-1.93	-1.19	-1.80	-1.35	-1.48	0.08
L Error (eV)**	0.01	0.04	0.00	0.08	0.04	0.21	0.04	0.11	0.03	0.11	0.16	0.17	0.07	
P Prediction 2/eV	-2.02	-1.43	-2.01	-2.15	-1.72	-1.40	-2.15	-1.78	-2.04	-1.08	-1.75	-1.15	-1.36	0.08
P Error (eV)**	0.13	-0.06	0.09	0.08	-0.03*	0.06	0.14	0.07	0.14	0.00	0.11	-0.03*	-0.05	
D prediction 1/eV	-2.11	-1.29	-1.89	-2.38	-1.58	-1.29	-2.38	-1.89	-2.12	-1.29	-1.58	-0.70	-1.58	0.21
T Error (eV)**	0.22	-0.20	-0.03	0.31	-0.17	-0.05	0.37	0.18	0.22	0.21	-0.06	-0.48	0.17	
R Prediction 2/eV	-2.12	-1.29	-1.89	-2.38	-1.60	-1.29	-2.38	-1.89	-2.12	-1.29	-1.60	-0.76	-1.60	0.20
R Error (eV)**	0.23	-0.20	-0.03	0.31	-0.15*	-0.05	0.37	0.18	0.22	0.21	-0.04	-0.42*	0.19	
Prediction 1/eV	-2.08	-1.44	-1.96	-2.17	-1.54	-1.38	-1.98	-1.94	-1.94	-1.18	-1.65	-1.13	-1.47	0.09
X Error (eV)**	0.19	-0.05	-0.04	0.10	-0.21	0.04	-0.03	0.23	0.04	0.10	0.01	-0.05	0.06	
G Prediction 2/eV	-2.04	-1.50	-1.93	-2.16	-1.75	-1.44	-1.90	-1.96	-1.99	-1.24	-1.65	-1.18	-1.54	0.08
G Error (eV)**	0.15	0.01	0.01	0.09	0.00*	0.10	-0.11	0.25	0.09	0.16	0.01	0.00*	0.13	
S prediction 1/eV	-1.76	-1.34	-1.71	-1.79	-1.50	-1.39	-1.81	-1.59	-1.69	-1.17	-1.56	-1.26	-1.35	0.15
V Error (eV)**	-0.13	-0.16	-0.21	-0.28	-0.25	0.05	-0.20	-0.12	-0.21	0.09	-0.08	0.08	-0.06	
R Prediction 2/eV	-1.99	-1.42	-1.93	-1.98	-1.75	-1.43	-2.03	-1.76	-1.87	-1.17	-1.70	-1.18	-1.46	0.05
R Error (eV)**	0.10	-0.07	0.01	-0.09	0.00*	0.09	0.02	0.05	-0.03	0.09	0.06	0.00*	0.05	

* These cases are part of the training set; therefore, small errors are expected.

** Error between DFT and predicted value