

Supporting Information:

**Catlas: an automated framework for catalyst
discovery demonstrated for direct syngas
conversion**

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1 Supplementary Information

1.1 111-likeness algorithm

The (1,1,1) surface facet characteristically is flat with all atoms identically having 6 neighbors. To characterize (1,1,1)-likeness the following algorithm was employed for all surfaces:

1. Find the maximum atomic radius R_{max} .
2. Find the atom with the highest z-coordinate position. This is the atom farthest out on the surface.
3. Find all atoms that lie within $0.5 * R_{max}$ of the highest z-coordinate position.
4. For every atom in (3) compute its coordination number with other atoms in (3) using JmolNN from pymatgen^{S1}
5. If all atoms have a coordination number of 6, then the surface is (1,1,1)-like. Otherwise it is not.

1.2 Validation DFT calculation details

DFT calculations were performed with the Vienna Ab Initio Simulation Package (VASP).^{S2-S6} The BEEF-vDW^{S7} functional was used for agreement with the microkinetic model (MKM) functional choice,^{S8} so dispersion corrections were included. Selective dynamics were not used, but a sub-sample of calculations performed with selective dynamics give the same conclusions. With these exceptions, all other parameters were set to be OC20-like.^{S9}

1.3 Selecting number of relaxations

Because the relaxation model selected directly predicts the pairwise forces rather than predicting the energies and getting the forces through the gradient, energy is not conserved. This results in the energy decreasing below the DFT energy in the many-relaxation limit.

To overcome this, we select the number of relaxations which minimizes the observed MAE on validation data. For *CO, this was 65 steps. As can be seen in Figure S1, this is in the domain where the MAE is well behaved, so there are incremental changes in the error with frame number.

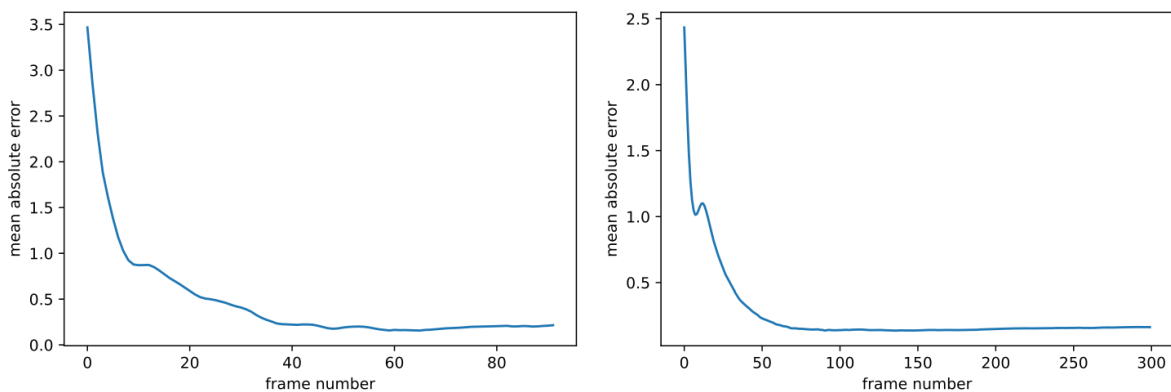


Figure S1: The MAE of *CO (left) and *OH (right) adsorption energies as a function of frame number.

1.4 All surfaces with near optimal selectivity

bulk id (MP) ^{S10}	bulk elements	slab miller indices	slab shift	top of slab?	$E_{ads,*OH}$	$E_{ads,*CO}$
mp-2260	[Fe, Pt]	(1, 0, 1)	0.250000	True	-0.034228	-1.783699
mp-1473	[Fe, W]	(0, 0, 1)	0.045254	False	-0.581535	-1.811932
mp-12798	[Ni, Pt]	(1, 1, 1)	0.166667	True	-0.013018	-1.767412
mp-1649	[Fe, Pt]	(1, 1, 1)	0.166667	True	-0.577986	-1.713270
mp-1670	[Mn, Pt]	(1, 0, 1)	0.250000	True	-0.154630	-1.644630
mp-1486	[Ni, Zn]	(1, 1, 0)	0.250000	True	0.103060	-1.537358
mp-1451	[Nb, Ni]	(1, 0, 0)	0.250000	True	-0.863065	-1.654895
mp-1451	[Nb, Ni]	(0, 1, 0)	0.000000	True	-0.444772	-1.496624
mp-12700	[Nb, Pt]	(0, 0, 1)	0.000000	True	-0.718271	-1.339915
mp-12700	[Nb, Pt]	(0, 0, 1)	0.248448	True	-0.910948	-1.345657
mp-12700	[Nb, Pt]	(0, 0, 1)	0.500000	True	-0.881095	-1.300059
mp-12700	[Nb, Pt]	(0, 0, 1)	0.248448	False	-0.711991	-1.308456
mp-1008349	[Co, Ni]	(1, 1, 1)	0.166667	True	-0.311042	-1.853170
mp-1018129	[Pt, W]	(1, 1, 0)	0.250000	True	-0.594530	-1.513859
mp-1007974	[Cr, Ni]	(1, 1, 1)	0.166667	True	-0.703715	-1.661447
mp-1078699	[Nb, Pt]	(1, 0, 0)	0.250000	True	-0.735216	-1.325013
mp-1078699	[Nb, Pt]	(0, 1, 0)	0.000000	True	-0.001919	-1.387082
mp-1062948	[Ni, V]	(1, 1, 0)	0.250000	True	-0.757680	-1.791392
mp-1079496	[Mo, Ni]	(1, 0, 0)	0.250000	True	-0.520703	-1.660118
mp-1079496	[Mo, Ni]	(0, 1, 0)	0.000000	True	-0.257014	-1.686100
mp-1018054	[Hf, Pt]	(1, 1, 1)	0.166667	True	-0.784960	-1.516634
mp-979980	[Pd, V]	(1, 0, 0)	0.000000	True	-0.396464	-1.503443
mp-979980	[Pd, V]	(0, 0, 1)	0.000000	True	-0.807857	-1.389312
mp-975834	[Mo, Ru]	(1, 0, 0)	0.000000	True	-0.531574	-1.773907
mp-974455	[Re, Ru]	(0, 0, 1)	0.124191	True	-0.239802	-1.686642
mp-974455	[Re, Ru]	(0, 0, 1)	0.124191	False	-0.293340	-1.715621
mp-999502	[Mo, Pt]	(0, 1, 0)	0.000000	True	-0.692265	-1.721138
mp-980200	[Rh, Zn]	(1, 0, 0)	0.000000	True	-0.303130	-1.147850
mp-980200	[Rh, Zn]	(1, 0, 0)	0.500000	True	-0.214180	-1.760503

mp-980200	[Rh, Zn]	(0, 0, 1)	0.000000	True	0.087079	-1.483808
mp-974625	[Re, Ru]	(1, 0, 0)	0.500000	True	-0.605735	-1.801409
mp-974625	[Re, Ru]	(0, 0, 1)	0.000000	True	-0.549948	-1.695066
mp-865960	[Co, Re]	(1, 0, 0)	0.500000	True	-0.659988	-1.835880
mp-865960	[Co, Re]	(0, 0, 1)	0.000000	True	-0.455686	-1.744242
mp-862604	[Ni, Re]	(1, 0, 0)	0.500000	True	-0.485833	-1.564701
mp-862604	[Ni, Re]	(0, 0, 1)	0.000000	True	-0.671528	-1.836270
mp-862586	[Pd, Re]	(1, 0, 0)	0.500000	True	-0.454122	-1.433507
mp-862589	[Pt, Re]	(1, 0, 0)	0.500000	True	-0.411939	-1.513011
mp-866161	[Rh, V]	(1, 0, 0)	0.000000	True	-0.270271	-1.654961
mp-867792	[Ir, Re]	(0, 0, 1)	0.000000	True	-0.192869	-1.873265
mp-865193	[Co, Pt]	(0, 0, 1)	0.000000	True	-0.273029	-1.760126
mp-867264	[Os, Re]	(0, 0, 1)	0.000000	True	-0.363004	-1.818342
mp-867141	[Os, Re]	(0, 0, 1)	0.000000	True	-0.113152	-1.784669
mp-865786	[Cr, Pd]	(1, 1, 1)	0.166667	True	-0.655093	-1.725830
mp-865045	[Mn, Ru]	(1, 0, 0)	0.500000	True	-0.681806	-1.833099
mp-865045	[Mn, Ru]	(0, 0, 1)	0.000000	True	-0.398070	-1.809611
mp-952	[Mo, Pt]	(1, 1, 0)	0.250000	True	-0.299522	-1.414902
mp-862655	[Ru, W]	(1, 0, 0)	0.000000	True	-0.491768	-1.799588
mp-971788	[Ru, V]	(1, 0, 0)	0.000000	True	-0.539803	-1.690420
mp-864735	[Ir, Mn]	(1, 0, 0)	0.500000	True	-0.459614	-1.874299
mp-862620	[Ir, Ru]	(0, 0, 1)	0.000000	True	-0.132057	-1.776171
mp-862630	[Re, Ru]	(1, 0, 0)	0.000000	True	-0.497756	-1.804558
mp-862630	[Re, Ru]	(0, 0, 1)	0.000000	True	-0.325783	-1.788968
mp-972220	[Pt, Ti]	(1, 0, 0)	0.000000	True	-0.058693	-1.442468
mp-972220	[Pt, Ti]	(0, 0, 1)	0.000000	True	-0.295566	-1.543388
mp-864889	[Zn, Zr]	(1, 0, 0)	0.000000	True	-0.571586	-1.426765
mp-866108	[Hf, Zn]	(1, 0, 0)	0.000000	True	-0.654416	-1.434227
mp-862260	[Sc, Zn]	(1, 0, 0)	0.000000	True	-0.780388	-1.013245
mp-891	[Ni, Ta]	(0, 1, 0)	0.000000	True	-0.574231	-1.503062
mp-12108	[Pt, V]	(1, 1, 0)	0.250000	True	-0.554510	-1.615371
mp-12083	[Cr, Ir]	(1, 1, 1)	0.166667	True	-0.041614	-1.739911
mp-12107	[Pt, Ti]	(1, 1, 1)	0.166667	True	-0.644000	-1.375335

mp-1187993	[Co, Zn]	(1, 0, 0)	0.000000	True	-0.152281	-1.657407
mp-1216329	[Fe, V]	(0, 0, 1)	0.150265	False	-0.342841	-1.787324
mp-1216675	[Mo, Ti]	(0, 0, 1)	0.084208	True	-0.828324	-1.587083
mp-1216323	[Mo, V]	(0, 0, 1)	0.250000	False	-0.719460	-1.467304
mp-1216231	[V, W]	(0, 0, 1)	0.250000	True	-0.581619	-1.541568
mp-1206750	[Cr, Pt]	(1, 0, 1)	0.250000	True	-0.604811	-1.541975
mp-1216486	[Rh, V]	(1, 1, 0)	0.125250	True	-0.267878	-1.619609
mp-1216486	[Rh, V]	(0, 0, 1)	0.250000	False	-0.570614	-1.854017
mp-1206704	[Mo, Pd]	(1, 1, 0)	0.250000	True	-0.483187	-1.613155
mp-1188129	[Pt, Zr]	(0, 0, 1)	0.125000	True	-0.368614	-1.545610
mp-1188129	[Pt, Zr]	(0, 0, 1)	0.125000	False	-0.734172	-1.545135
mp-569250	[Ir, V]	(1, 1, 0)	0.000000	True	-0.828832	-1.789054
mp-568711	[Pd, V]	(1, 1, 1)	0.166667	True	-0.929191	-1.373539
mp-372	[Pt, V]	(1, 1, 1)	0.166667	True	-0.686545	-1.267434
mp-601848	[Co, Fe]	(1, 1, 0)	0.125000	False	-0.566689	-1.670413
mp-784631	[Cr, Ni]	(1, 1, 0)	0.250000	True	-0.501827	-1.788598
mp-569594	[Fe, Mo]	(0, 0, 1)	0.143018	True	-0.671857	-1.732608
mp-569594	[Fe, Mo]	(0, 0, 1)	0.045392	False	-0.624289	-1.764790
mp-636328	[Pd, Ti]	(1, 1, 1)	0.166667	True	-0.904211	-1.368673
mp-567747	[Co, Mo]	(0, 0, 1)	0.141359	True	-0.711523	-1.673207
mp-567747	[Co, Mo]	(0, 0, 1)	0.045498	False	-0.172400	-1.705292
mp-784630	[Mo, Ni]	(1, 1, 0)	0.250000	True	-0.503541	-1.730431
mp-429	[Ni, Zn]	(1, 1, 0)	0.250000	True	-0.064436	-1.670468
mp-429	[Ni, Zn]	(1, 0, 1)	0.250000	True	0.141199	-1.496193
mp-569708	[Pt, Ti]	(0, 0, 1)	0.071531	True	-0.309840	-1.421662
mp-569708	[Pt, Ti]	(0, 0, 1)	0.214738	True	-0.633384	-1.461240
mp-569708	[Pt, Ti]	(0, 0, 1)	0.357679	True	-0.278580	-1.455170
mp-569708	[Pt, Ti]	(0, 0, 1)	0.500000	True	-0.639207	-1.469249
mp-569708	[Pt, Ti]	(0, 0, 1)	0.071531	False	-0.632338	-1.344598
mp-569708	[Pt, Ti]	(0, 0, 1)	0.214738	False	-0.646107	-1.366716
mp-569708	[Pt, Ti]	(0, 0, 1)	0.357679	False	-0.616021	-1.366716
mp-481	[Pt, Sc]	(1, 1, 1)	0.166667	True	-0.371900	-1.716151
mp-11798	[Fe, Pt]	(1, 1, 1)	0.000000	True	-0.547112	-1.684698

mp-1180	[Mn, Pt]	(1, 1, 1)	0.166667	True	-0.008136	-1.852638
mp-1187241	[Ir, Ta]	(1, 0, 0)	0.000000	True	-0.190298	-1.876457
mp-1183654	[Cd, Pt]	(1, 0, 0)	0.500000	True	-0.036801	-1.220765
mp-1186060	[Mn, Os]	(0, 0, 1)	0.000000	True	-0.156880	-1.808685
mp-1185931	[Mn, Pt]	(1, 0, 0)	0.500000	True	-0.452302	-1.450316
mp-1187531	[Ti, Zn]	(1, 0, 0)	0.000000	True	-0.479079	-1.445411
mp-1186230	[Nb, Rh]	(1, 0, 0)	0.000000	True	-0.262426	-1.645294
mp-1185935	[Mn, Os]	(0, 0, 1)	0.000000	True	-0.892616	-1.724480
mp-1183749	[Cr, Ir]	(0, 0, 1)	0.000000	True	-0.038867	-1.831886
mp-1185970	[Co, Mn]	(1, 0, 0)	0.500000	True	-0.688333	-1.826474
mp-1186926	[Rh, Ru]	(0, 0, 1)	0.000000	True	-0.204907	-1.780415
mp-1183837	[Co, Ni]	(0, 0, 1)	0.000000	True	-0.278816	-1.853478
mp-1186923	[Re, Rh]	(1, 0, 0)	0.500000	True	-0.460102	-1.580108
mp-1187948	[Ni, Zn]	(1, 0, 0)	0.500000	True	-0.019384	-1.362913
mp-1187948	[Ni, Zn]	(0, 0, 1)	0.000000	True	0.058052	-1.335319
mp-1186902	[Ir, Re]	(1, 1, 1)	0.166667	True	-0.554933	-1.715087
mp-11549	[Pd, V]	(1, 1, 0)	0.250000	True	-0.797452	-1.564889
mp-11531	[Ni, V]	(1, 1, 0)	0.250000	True	-0.756335	-1.801121
mp-1082	[Ir, V]	(1, 1, 1)	0.166667	True	-0.234828	-1.843476
mp-11506	[Mo, Ni]	(1, 0, 0)	0.250000	True	-0.544527	-1.682024
mp-11506	[Mo, Ni]	(0, 1, 0)	0.000000	True	-0.241762	-1.676790
mp-11482	[Ir, Mo]	(0, 0, 1)	0.000000	True	-0.135846	-1.724527
mp-11501	[Mn, Ni]	(1, 1, 1)	0.166667	True	-0.320767	-1.861347
mp-11514	[Nb, Pt]	(1, 1, 0)	0.250000	True	-0.782335	-1.344121
mp-1104334	[Co, Nb]	(0, 0, 1)	0.046010	False	-0.289097	-1.841525
mp-1104548	[Co, Ta]	(0, 0, 1)	0.044969	False	-0.288939	-1.857507
mp-1105911	[Pd, Ti]	(0, 0, 1)	0.125000	True	-0.700381	-1.501689
mp-1105911	[Pd, Ti]	(0, 0, 1)	0.125000	False	-0.915475	-1.544555
mp-11456	[Hf, Pt]	(0, 0, 1)	0.125000	True	-0.390415	-1.501042
mp-11456	[Hf, Pt]	(0, 0, 1)	0.125000	False	-0.775310	-1.519178
mp-12546	[Cu, Ti]	(0, 1, 0)	0.000000	True	-0.994866	-1.432420
mp-12585	[Cr, Rh]	(1, 1, 1)	0.166667	True	-0.361569	-1.780942
mp-1226229	[Cr, Ir]	(1, 0, 0)	0.000000	True	-1.013624	-1.369588

mp-1220327	[Mo, Nb]	(0, 0, 1)	0.250000	False	-0.960246	-1.662498
mp-1220023	[Os, Ru]	(0, 0, 1)	0.250000	True	-0.083692	-1.813679
mp-1217895	[Mo, Ta]	(0, 0, 1)	0.250000	False	-0.960685	-1.606262
mp-1219503	[Rh, Ru]	(1, 0, 0)	0.333333	False	0.021036	-1.718800
mp-1219522	[Rh, Ru]	(0, 0, 1)	0.032800	True	-0.173893	-1.867572
mp-1221420	[Mo, Pt]	(0, 1, 0)	0.250000	True	-0.853504	-1.700851
mp-1225078	[Fe, Ni]	(0, 0, 1)	0.124845	True	0.026343	-1.637069
mp-1219539	[Re, Rh]	(1, 0, 0)	0.000000	False	-0.822292	-1.786918
mp-1219539	[Re, Rh]	(0, 0, 1)	0.124477	False	-0.291705	-1.702479
mp-1219539	[Re, Rh]	(0, 0, 1)	0.374477	False	-0.239763	-1.777312
mp-1219533	[Ir, Re]	(1, 0, 0)	0.333333	False	-0.715015	-1.801965
mp-1219509	[Os, Re]	(1, 0, 0)	0.333333	False	-0.833168	-1.773237
mp-1219509	[Os, Re]	(0, 0, 1)	0.250000	True	-0.322936	-1.809230
mp-1219535	[Ir, Re]	(0, 0, 1)	0.041055	True	-0.194174	-1.786659
mp-30866	[Rh, W]	(1, 0, 0)	0.000000	True	-0.249425	-1.670903
mp-30745	[Ir, W]	(0, 0, 1)	0.000000	True	-0.538285	-1.687359
mp-2728	[Ir, Mn]	(1, 0, 1)	0.250000	True	-0.298498	-1.599189
mp-2515	[Cr, Pt]	(1, 1, 1)	0.166667	True	-0.389627	-1.617300
mp-30850	[Pt, Ta]	(0, 1, 0)	0.000000	True	-0.194773	-1.385019
mp-30858	[Pt, Zr]	(1, 1, 1)	0.166667	True	-0.774167	-1.583935
mp-30842	[Pd, Zr]	(0, 0, 1)	0.125000	True	-0.886063	-1.437452
mp-2403	[Pt, Y]	(1, 1, 1)	0.166667	True	-0.286169	-1.858475
mp-2677	[Pd, Sc]	(1, 1, 1)	0.166667	True	-0.643742	-1.824384

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