Supplementary information

Rational ensemble design of alloy catalysts for selective ammonia oxidation based on machine learning

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1. Computational sets

High-throughput density functional theory (DFT) calculation is performed via VASP code. The exchange and correlation energy are in the form of generalized gradient approximation (GGA) with Perdew−Burke−Ernzerhof (PBE). Projector augmented wave (PAW) method is adopted to describe the electron-ion interactions. The Gaussian broadening with a width of 0.05 eV is used for the integration of the first Brillouin zone. The cutoff energy of 400 eV and Monkhorst−Pack k-meshes of 3×3×1 are needed for the calculation of binding energy at low-index fates of metallic catalysts. The bottom two layers of surface models are frozen and the top two layers and adsorption species are relaxed until the Hellmann−Feynman force is smaller than 0.05 eV/Å. The climbing-image nudged elastic band (CI-NEB) method is performed to locate the reaction barriers of elementary steps via inserting six intermediate images between initial and final configurations.

Benchmark calculation is also performed on the ensembles with relatively weak binding ability to check the effect of weak interaction. Ag_Au_111_1 is selected as the representative with weak binding ability of intermediates to perform Van der Waals corrected calculation of binding energy and the comparison of binding energy with and without Van der Waals (VDW) correction ($E_{b(vdw)}$ and E_b) are shown in Table S1. It is found that the difference of binding energy with and without VDW correction are below 0.25 eV for the ensembles with weak binding ability, which the weak influence of Van der Waals interaction on the binding energies of intermediates in NH_3-SCO process. Similarly, the VDW interaction is also not considered in previous study about NH_3-SCO on metal catalysts.[1-4] Based that, weak interaction for adsorption behavior is ignored for accelerating calculation of binding energy in the study.

Table S1. The binding energies of intermediates with and without Van der Waals correction ($E_{b(vdw)}$ and E_b) on the ensembles Ag_Au_111_1 as the representative with weak binding ability of intermediates.

Species	*NH_3*	*NH_2*	*NH*	*N*	*O*	*OH*	*H*
$E_{b(vdw)}$ (eV)	-0.56	-1.80	-2.47	-2.32	-0.29	-2.55	-2.16
E_b (eV)	-0.319	-1.546	-2.259	-2.161	-0.165	-2.36	-2.086
$E_{b(vdw)}$-E_b	-0.25	-0.25	-0.21	-0.16	-0.12	-0.19	-0.07

2. The stability of ensembles

The stability of ensemble configurations is evaluated via the formation energy of ensembles (E_f),[5] as followed:

$$E_f = -[E_{AB} - E_A - n_B(E_{B-atom} - E_{A-bulk})]/n_B$$

Where, E_{AB}, E_A, $E_{A\text{-}bulk}$, *and* $E_{B\text{-}atom}$ are the total energies of the AB slab, clean A slab, bulk A atom (per atom) and isolated B atom, respectively and n_B is the number of B atoms. Note that A and B are for the host and doped elements. Taking an example, as for Pd_Cu_111_1 ensemble, A and B represent Pd and Cu atoms and E_{AB}, E_A, $E_{A\text{-}bulk}$, *and* $E_{B\text{-}atom}$ are for the energies of Pd_Cu_111_1 ensemble, Pd(111), per Pd atom in bulk and isolated Cu atom, respectively and n_B is the number of doped Cu atoms in

Pd_Cu_111_1 ensemble. The related calculated E_f for all ensembles are shown in Table S2.

The surface energy (E_{surf}) of surface ensemble models are calculated to evaluated the stability.[6,7] The formula is followed:

$$E_{surf} = \frac{E_{AB} - n_A E_{A-bulk} - n_B E_{B-bulk}}{2S}$$

Where, $E_{AB,}$ *is* the total energy of surface ensemble models (AB) and $E_{A\text{-}bulk,}$ *and* $E_{B\text{-}bulk}$ are the energy of per A and B atoms in bulk. n_A and n_B are the numbers of A and B atoms in the surface ensemble models. S is the area of the surface ensemble model.

Calculated formation energies and surface energies of different ensemble models are shown in Table S2. It is found that the ensemble configurations all exhibit the positive E_f, which demonstrates the formation of these ensembles should be an exothermic process. On the other hand, Ag-, Au-, Cu-, Pd- and Pt-based ensemble models possess a surface energy of below 2.00 J/m^2 and surface energy of Ir- and Rh-based surface models are larger than other systems. Overall, surface energies of all systems are smaller than 3.00 J/m^2 and the surface energies of surface-doped systems are generally near to the that of corresponding pristine systems.[7] Based on the theoretical calculation on surface energy and formation energy of ensembles, we believe that the ensembles should be stable. Note that two kinds of trimer configurations are calculated and the two show the similar formation energy and surface energy and thus the two kinds of trimers are viewed as the same configuration for the simplification in our study.

Table S2. The formation energy of ensembles (E_f) (eV) of ensembles and surface energy (E_{surf}) (J/m^2) for alloy systems.

Ensembles	E_f **(eV)**	E_{surf} **(J/m^2)**	***Ensembles***	E_f **(eV)**	E_{surf} **(J/m^2)**
Ag_Au_100_1	3.229	0.787	Ag_Au_111_1	3.247	0.729
Ag_Au_100_1L	3.131	0.712	Ag_Au_111_1L	3.154	0.605
Ag_Au_100_2	3.213	0.770	Ag_Au_111_2	3.244	0.700
Ag_Au_100_4	3.190	0.741	Ag_Au_111_3_0	3.229	0.677
Ag_Cu_100_1	3.006	0.858	Ag_Au_111_3_1	3.230	0.676
Ag_Cu_100_1L	2.978	1.283	Ag_Cu_111_1	3.007	0.826
Ag_Cu_100_2	2.994	0.910	Ag_Cu_111_1L	2.945	1.434
Ag_Cu_100_4	2.984	1.017	Ag_Cu_111_2	3.009	0.892
Ag_Ir_100_1	5.103	1.039	Ag_Cu_111_3_0	3.007	0.959
Ag_Ir_100_1L	5.257	2.746	Ag_Cu_111_3_1	3.007	0.959
Ag_Ir_100_2	5.350	1.219	Ag_Ir_111_1	5.117	1.066
Ag_Ir_100_4	5.615	1.521	Ag_Ir_111_1L	5.823	2.643
Ag_Pd_100_1	3.669	0.814	Ag_Ir_111_2	5.468	1.276
Ag_Pd_100_1L	3.446	1.073	Ag_Ir_111_3_0	5.593	1.482
Ag_Pd_100_2	3.594	0.836	Ag_Ir_111_3_1	5.590	1.483
Ag_Pd_100_4	3.559	0.879	Ag_Pd_111_1	3.577	0.781
Ag_Pt_100_1	5.084	0.849	Ag_Pd_111_1L	3.494	1.053
Ag_Pt_100_1L	4.851	1.400	Ag_Pd_111_2	3.491	0.826

Ag_Pt_100_2	5.014	0.906	Ag_Pd_111_3_0	3.480	0.863
Ag_Pt_100_4	4.970	1.022	Ag_Pd_111_3_1	3.483	0.862
Ag_Rh_100_1	4.569	0.951	Ag_Pt_111_1	5.070	0.817
Ag_Rh_100_1L	4.519	2.145	Ag_Pt_111_1L	5.114	1.223
Ag_Rh_100_2	4.628	1.082	Ag_Pt_111_2	5.026	0.887
Ag_Rh_100_4	4.699	1.328	Ag_Pt_111_3_0	5.073	0.931
Au_Ag_100_1	2.592	0.855	Ag_Pt_111_3_1	5.080	0.928
Au_Ag_100_1L	2.575	0.811	Ag_Rh_111_1	4.461	0.966
Au_Ag_100_2	2.648	0.836	Ag_Rh_111_1L	4.773	2.227
Au_Ag_100_4	2.626	0.819	Ag_Rh_111_2	4.612	1.130
Au_Cu_100_1	3.243	0.887	Ag_Rh_111_3_0	4.700	1.279
Au_Cu_100_1L	3.213	1.118	Ag_Rh_111_3_1	4.695	1.281
Au_Cu_100_2	3.239	0.913	Au_Ag_111_1	2.591	0.692
Au_Cu_100_4	3.236	0.966	Au_Ag_111_1L	2.501	0.725
Au_Ir_100_1	5.180	1.084	Au_Ag_111_2	2.584	0.684
Au_Ir_100_1L	5.325	2.728	Au_Ag_111_3_0	2.571	0.681
Au_Ir_100_2	5.376	1.266	Au_Ag_111_3_1	2.572	0.681
Au_Ir_100_4	5.580	1.587	Au_Cu_111_1	3.190	0.743
Au_Pd_100_1	3.623	0.873	Au_Cu_111_1L	3.021	1.280
Au_Pd_100_1L	3.492	1.083	Au_Cu_111_2	3.172	0.789
Au_Pd_100_2	3.592	0.891	Au_Cu_111_3_0	3.138	0.846
Au_Pd_100_4	3.588	0.921	Au_Cu_111_3_1	3.153	0.840
Au_Pt_100_1	4.855	0.927	Au_Ir_111_1	5.159	1.001
Au_Pt_100_1L	4.791	1.507	Au_Ir_111_1L	5.731	2.690
Au_Pt_100_2	4.840	0.995	Au_Ir_111_2	5.476	1.213
Au_Pt_100_4	4.849	1.125	Au_Ir_111_3_0	5.593	1.421
Au_Rh_100_1	4.706	0.991	Au_Ir_111_3_1	5.598	1.419
Au_Rh_100_1L	4.667	2.056	Au_Pd_111_1	3.431	0.743
Au_Rh_100_2	4.753	1.110	Au_Pd_111_1L	3.423	1.081
Au_Rh_100_4	4.773	1.349	Au_Pd_111_2	3.423	0.786
Cu_Ag_100_1	2.690	1.429	Au_Pd_111_3_0	3.422	0.829
Cu_Ag_100_1L	2.446	1.541	Au_Pd_111_3_1	3.426	0.827
Cu_Ag_100_2	2.650	1.417	Au_Pt_111_1	4.762	0.801
Cu_Ag_100_4	2.611	1.403	Au_Pt_111_1L	4.950	1.365
Cu_Au_100_1	3.583	1.377	Au_Pt_111_2	4.804	0.889
Cu_Au_100_1L	3.101	1.363	Au_Pt_111_3_0	4.870	0.956
Cu_Au_100_2	3.509	1.322	Au_Pt_111_3_1	4.866	0.957
Cu_Au_100_4	3.428	1.236	Au_Rh_111_1	4.563	0.893
Cu_Ir_100_1	6.340	1.587	Au_Rh_111_1L	4.762	2.176
Cu_Ir_100_1L	6.534	2.435	Au_Rh_111_2	4.716	1.042
Cu_Ir_100_2	6.459	1.690	Au_Rh_111_3_0	4.779	1.186
Cu_Ir_100_4	6.518	1.897	Au_Rh_111_3_1	4.771	1.190
Cu_Pd_100_1	4.152	1.395	Ir_Ag_111_1	2.243	2.591
Cu_Pd_100_1L	3.799	1.369	Ir_Ag_111_1L	2.618	2.407

Cu_Pd_100_2	4.058	1.363	Ir_Ag_111_2	2.197	2.649
Cu_Pd_100_4	3.999	1.307	Ir_Ag_111_3_0	2.227	2.686
Cu_Pt_100_1	5.857	1.402	Ir_Ag_111_3_1	2.195	2.701
Cu_Pt_100_1L	5.487	1.452	Ir_Au_111_1	3.050	2.544
Cu_Pt_100_2	5.769	1.376	Ir_Au_111_1L	3.210	2.288
Cu_Pt_100_4	5.703	1.336	Ir_Au_111_2	3.019	2.550
Cu_Rh_100_1	5.471	1.517	Ir_Au_111_3_0	3.015	2.553
Cu_Rh_100_1L	5.463	2.052	Ir_Au_111_3_1	2.993	2.564
Cu_Rh_100_2	5.477	1.581	Ir_Cu_111_1	3.348	2.569
Cu_Rh_100_4	5.436	1.733	Ir_Cu_111_1L	3.609	2.376
Ir_Ag_100_1	2.838	2.922	Ir_Cu_111_2	3.294	2.609
Ir_Ag_100_1L	3.039	2.405	Ir_Cu_111_3_0	3.327	2.624
Ir_Ag_100_2	2.855	2.880	Ir_Cu_111_3_1	3.295	2.640
Ir_Ag_100_4	2.874	2.792	Ir_Pd_111_1	3.836	2.530
Ir_Au_100_1	3.503	2.903	Ir_Pd_111_1L	4.012	2.147
Ir_Au_100_1L	3.584	2.366	Ir_Pd_111_2	3.838	2.513
Ir_Au_100_2	3.504	2.847	Ir_Pd_111_3_0	3.853	2.489
Ir_Au_100_4	3.479	2.746	Ir_Pd_111_3_1	3.853	2.489
Ir_Cu_100_1	3.807	2.922	Ir_Pt_111_1	5.780	2.501
Ir_Cu_100_1L	4.063	2.347	Ir_Pt_111_1L	5.842	2.043
Ir_Cu_100_2	3.857	2.873	Ir_Pt_111_2	5.786	2.453
Ir_Cu_100_4	3.904	2.763	Ir_Pt_111_3_0	5.793	2.402
Ir_Pd_100_1	4.248	2.898	Ir_Pt_111_3_1	5.794	2.402
Ir_Pd_100_1L	4.322	2.328	Ir_Rh_111_1	6.027	2.536
Ir_Pd_100_2	4.285	2.828	Ir_Rh_111_1L	6.033	2.441
Ir_Pd_100_4	4.291	2.694	Ir_Rh_111_2	6.024	2.526
Ir_Pt_100_1	5.982	2.901	Ir_Rh_111_3_0	6.024	2.516
Ir_Pt_100_1L	6.029	2.381	Ir_Rh_111_3_1	6.023	2.516
Ir_Pt_100_2	5.998	2.839	Cu_Ag_111_1	2.537	1.400
Ir_Pt_100_4	6.007	2.713	Cu_Ag_111_1L	2.178	1.956
Ir_Rh_100_1	6.249	2.925	Cu_Ag_111_2	2.501	1.410
Ir_Rh_100_1L	6.228	2.671	Cu_Ag_111_3_0	2.470	1.430
Ir_Rh_100_2	6.250	2.890	Cu_Ag_111_3_1	2.470	1.430
Ir_Rh_100_4	6.245	2.823	Cu_Au_111_1	3.538	1.311
Pd_Ag_100_1	2.894	1.439	Cu_Au_111_1L	2.748	1.857
Pd_Ag_100_1L	2.912	1.078	Cu_Au_111_2	3.456	1.249
Pd_Ag_100_2	2.898	1.395	Cu_Au_111_3_0	3.381	1.213
Pd_Ag_100_4	2.898	1.308	Cu_Au_111_3_1	3.381	1.213
Pd_Au_100_1	3.504	1.427	Cu_Ir_111_1	6.478	1.559
Pd_Au_100_1L	3.450	1.047	Cu_Ir_111_1L	6.912	2.101
Pd_Au_100_2	3.490	1.376	Cu_Ir_111_2	6.665	1.647
Pd_Au_100_4	3.472	1.279	Cu_Ir_111_3_0	6.656	1.774
Pd_Cu_100_1	3.639	1.464	Cu_Ir_111_3_1	6.661	1.771
Pd_Cu_100_1L	3.641	1.326	Cu_Pd_111_1	3.962	1.362

Pd_Cu_100_2	3.637	1.448	Cu_Pd_111_1L	3.737	1.393
Pd_Cu_100_4	3.637	1.414	Cu_Pd_111_2	3.926	1.333
Pd_Ir_100_1	6.456	1.583	Cu_Pd_111_3_0	3.922	1.300
Pd_Ir_100_1L	6.450	2.402	Cu_Pd_111_3_1	3.921	1.300
Pd_Ir_100_2	6.500	1.675	Cu_Pt_111_1	5.852	1.337
Pd_Ir_100_4	6.507	1.865	Cu_Pt_111_1L	5.540	1.319
Pd_Pt_100_1	5.414	1.490	Cu_Pt_111_2	5.834	1.279
Pd_Pt_100_1L	5.378	1.595	Cu_Pt_111_3_0	5.854	1.205
Pd_Pt_100_2	5.415	1.498	Cu_Pt_111_3_1	5.851	1.207
Pd_Pt_100_4	5.406	1.519	Cu_Rh_111_1	5.396	1.504
Pd_Rh_100_1	5.338	1.553	Cu_Rh_111_1L	5.595	1.990
Pd_Rh_100_1L	5.360	2.098	Cu_Rh_111_2	5.504	1.566
Pd_Rh_100_2	5.362	1.618	Cu_Rh_111_3_0	5.500	1.650
Pd_Rh_100_4	5.367	1.752	Cu_Rh_111_3_1	5.510	1.645
Pt_Ag_100_1	2.930	1.793	Pt_Ag_111_1	2.627	1.646
Pt_Ag_100_1L	2.978	1.374	Pt_Ag_111_1L	2.765	1.331
Pt_Ag_100_2	2.949	1.742	Pt_Ag_111_2	2.684	1.613
Pt_Ag_100_4	2.956	1.642	Pt_Ag_111_3_0	2.743	1.562
Pt_Au_100_1	3.387	1.799	Pt_Ag_111_3_1	2.720	1.572
Pt_Au_100_1L	3.435	1.427	Pt_Au_111_1	3.186	1.639
Pt_Au_100_2	3.391	1.757	Pt_Au_111_1L	3.267	1.340
Pt_Au_100_4	3.392	1.675	Pt_Au_111_2	3.207	1.609
Pt_Cu_100_1	3.686	1.817	Pt_Au_111_3_0	3.224	1.574
Pt_Cu_100_1L	3.833	1.490	Pt_Au_111_3_1	3.230	1.572
Pt_Cu_100_2	3.741	1.782	Pt_Cu_111_1	3.508	1.66
Pt_Cu_100_4	3.782	1.707	Pt_Cu_111_1L	3.553	1.576
Pt_Ir_100_1	6.667	1.915	Pt_Cu_111_2	3.545	1.646
Pt_Ir_100_1L	6.648	2.545	Pt_Cu_111_3_0	3.571	1.626
Pt_Ir_100_2	6.680	1.989	Pt_Cu_111_3_1	3.592	1.616
Pt_Ir_100_4	6.667	2.144	Pt_Ir_111_1	6.666	1.764
Pt_Pd_100_1	3.940	1.816	Pt_Ir_111_1L	6.765	2.446
Pt_Pd_100_1L	3.932	1.635	Pt_Ir_111_2	6.700	1.856
Pt_Pd_100_2	3.941	1.792	Pt_Ir_111_3_0	6.719	1.944
Pt_Pd_100_4	3.940	1.745	Pt_Ir_111_3_1	6.7300	1.939
Pt_Rh_100_1	5.694	1.869	Pt_Pd_111_1	3.791	1.654
Pt_Rh_100_1L	5.664	2.138	Pt_Pd_111_1L	3.806	1.561
Pt_Rh_100_2	5.693	1.899	Pt_Pd_111_2	3.799	1.642
Pt_Rh_100_4	5.686	1.962	Pt_Pd_111_3_0	3.804	1.630
Rh_Ag_100_1	2.878	2.468	Pt_Pd_111_3_1	3.804	1.630
Rh_Ag_100_1L	3.020	1.966	Pt_Rh_111_1	5.612	1.715
Rh_Ag_100_2	2.878	2.425	Pt_Rh_111_1L	5.579	2.176
Rh_Ag_100_4	2.891	2.332	Pt_Rh_111_2	5.611	1.767
Rh_Au_100_1	3.643	2.437	Pt_Rh_111_3_0	5.606	1.821
Rh_Au_100_1L	3.625	1.861	Pt_Rh_111_3_1	5.605	1.822

Rh_Au_100_2	3.625	2.367	Pd_Ag_111_1	2.852	1.471
Rh_Au_100_4	3.596	2.237	Pd_Ag_111_1L	2.825	1.102
Rh_Cu_100_1	3.798	2.474	Pd_Ag_111_2	2.875	1.413
Rh_Cu_100_1L	3.934	2.027	Pd_Ag_111_3_0	2.888	1.353
Rh_Cu_100_2	3.808	2.435	Pd_Ag_111_3_1	2.896	1.350
Rh_Cu_100_4	3.840	2.342	Pd_Au_111_1	3.588	1.436
Rh_Ir_100_1	7.181	2.531	Pd_Au_111_1L	3.403	1.007
Rh_Ir_100_1L	7.155	2.717	Pd_Au_111_2	3.573	1.355
Rh_Ir_100_2	7.177	2.552	Pd_Au_111_3_0	3.556	1.280
Rh_Ir_100_4	7.170	2.596	Pd_Au_111_3_1	3.558	1.279
Rh_Pd_100_1	4.115	2.465	Pd_Cu_111_1	3.676	1.493
Rh_Pd_100_1L	4.157	2.047	Pd_Cu_111_1L	3.566	1.416
Rh_Pd_100_2	4.127	2.416	Pd_Cu_111_2	3.675	1.465
Rh_Pd_100_4	4.133	2.317	Pd_Cu_111_3_0	3.665	1.441
Rh_Pt_100_1	5.935	2.458	Pd_Cu_111_3_1	3.673	1.438
Rh_Pt_100_1L	5.919	2.042	Pd_Ir_111_1	6.588	1.637
Rh_Pt_100_2	5.931	2.404	Pd_Ir_111_1L	6.746	2.342
Rh_Pt_100_4	5.928	2.299	Pd_Ir_111_2	6.672	1.727
			Pd_Ir_111_3_0	6.689	1.822
			Pd_Ir_111_3_1	6.714	1.810
			Pd_Pt_111_1	5.534	1.515
			Pd_Pt_111_1L	5.538	1.453
			Pd_Pt_111_2	5.540	1.506
			Pd_Pt_111_3_0	5.543	1.497
			Pd_Pt_111_3_1	5.543	1.496
			Pd_Rh_111_1	5.357	1.613
			Pd_Rh_111_1L	5.451	2.219
			Pd_Rh_111_2	5.394	1.694
			Pd_Rh_111_3_0	5.414	1.771
			Pd_Rh_111_3_1	5.426	1.765
			Rh_Ag_111_1	2.526	2.389
			Rh_Ag_111_1L	2.707	2.119
			Rh_Ag_111_2	2.486	2.401
			Rh_Ag_111_3_0	2.477	2.411
			Rh_Ag_111_3_1	2.508	2.396
			Rh_Au_111_1	3.432	2.325
			Rh_Au_111_1L	3.340	1.938
			Rh_Au_111_2	3.381	2.276
			Rh_Au_111_3_0	3.339	2.240
			Rh_Au_111_3_1	3.360	2.230
			Rh_Cu_111_1	3.548	2.381
			Rh_Cu_111_1L	3.647	2.161
			Rh_Cu_111_2	3.511	2.383
			Rh_Cu_111_3_0	3.497	2.386

	Rh_Cu_111_3_1	3.522	2.375
	Rh_Ir_111_1	7.338	2.391
	Rh_Ir_111_1L	7.317	2.428
	Rh_Ir_111_2	7.328	2.395
	Rh_Ir_111_3_0	7.321	2.401
	Rh_Ir_111_3_1	7.321	2.401
	Rh_Pd_111_1	3.947	2.355
	Rh_Pd_111_1L	3.988	2.016
	Rh_Pd_111_2	3.935	2.324
	Rh_Pd_111_3_0	3.933	2.292
	Rh_Pd_111_3_1	3.935	2.291
	Rh_Pt_111_1	5.927	2.319
	Rh_Pt_111_1L	5.877	1.825
	Rh_Pt_111_2	5.910	2.254
	Rh_Pt_111_3_0	5.899	2.191
	Rh_Pt_111_3_1	5.899	2.191

3. Feature design for binding energy prediction

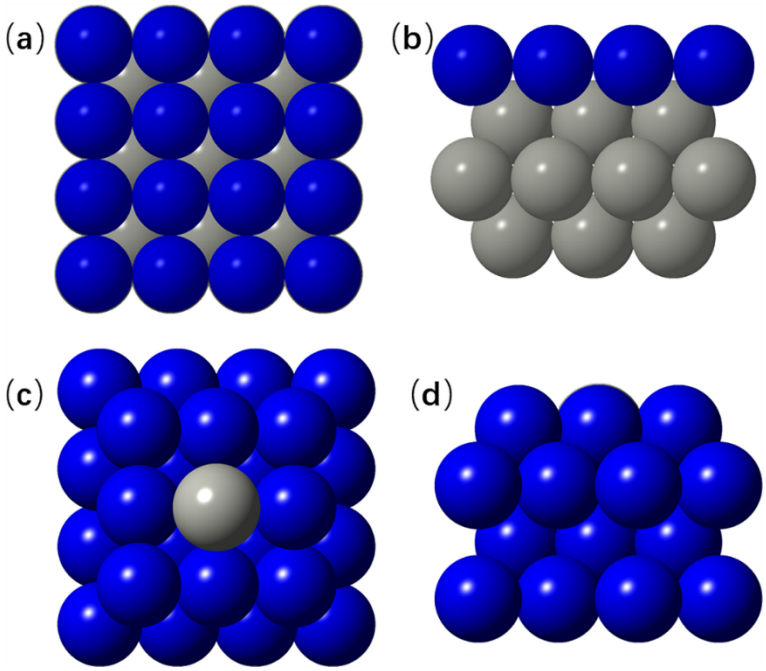

Fig. S1. The top and side views of Pd_Cu_100_1L (a, b) and Cu_Pd_100_1 (c, d).

Table S3. The values of surface and subsurface features for Pd_Cu_100_1L and Cu_Pd_100_1.

Features	Pd_Cu_100_1L	Cu_Pd_100_1
ave_elec_surf	11.0	10.89

ave_rad_surf	1.32	1.33
ave_elec_sub	10.0	11.0
ave_rad_sub	1.39	1.32

4. Ensemble machine learning on binding energy prediction

Table S4. The hyperparameter ranges and obtained hyperparameters of best models after hyperparameter optimization.

Method	Hyperparameter range	Best Model
RFR	{'n_estimators': [300,400,500,600,700,800], 'max_depth': [15,16,17,18,19,20,21,22]}	{'n_estimators':400,' max_depth':17}
ETR	{'n_estimators': [300,400,500,600,700,800], 'max_depth': [15,16,17,18,19,20,21,22]}	{'n_estimators':400, 'max_depth':21}
GBR	{'n_estimators': [900,1000,1100,1200,1300,1400,1500], 'max_depth': [2,3,4,5,6,7,8,9], 'learning_rate': [0.1]}	{'n_estimators':1100, 'max_depth':4, 'learning_rate': [0.1]}

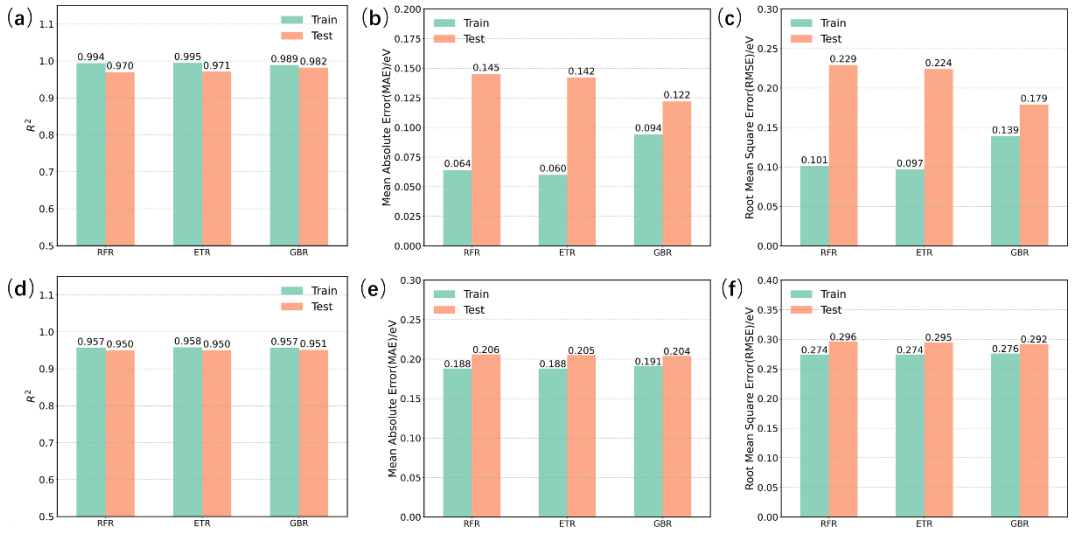

Fig. S2. R^2, MAE and RMSE of train and test sets for RFR, ETR, and GBR models with surface features ((a), (b), (c)) and without surface features ((d), (e), (f)).

5. Clustering analysis

Table S5. The original data set for the clustering analysis on catalytic performance.

$E(NH_3)$	$E(NH_2)$	E(NH)	E(N)	E(O)	E(OH)	E(H)	Systems
-0.394	-1.264	-2.694	-2.851	-0.649	-2.748	-2.093	Ag_Au_100_1
-0.542	-1.914	-3.206	-3.459	-1.304	-3.201	-2.160	Ag_Cu_100_1
-0.458	-1.590	-3.012	-3.271	-0.920	-2.848	-2.383	Ag_Pd_100_1
-0.447	-1.924	-3.165	-3.636	-0.979	-2.764	-2.704	Ag_Pt_100_1
-1.025	-2.833	-3.944	-5.065	-1.951	-3.418	-3.182	Ag_Ir_100_1
-0.892	-2.436	-3.632	-4.438	-1.581	-3.154	-2.740	Ag_Rh_100_1

-0.684	-2.127	-2.693	-2.754	-0.272	-2.436	-2.265	Au_Ag_100_1
-0.841	-2.446	-2.802	-2.959	-0.627	-2.814	-2.283	Au_Cu_100_1
-0.706	-2.313	-2.766	-3.028	-0.271	-2.410	-2.518	Au_Pd_100_1
-0.812	-2.600	-3.047	-3.575	-0.646	-2.534	-2.740	Au_Pt_100_1
-1.298	-3.097	-3.924	-4.924	-1.721	-3.270	-3.108	Au_Ir_100_1
-1.114	-2.796	-3.442	-4.387	-1.223	-2.844	-2.742	Au_Rh_100_1
-0.545	-1.795	-3.811	-4.236	-1.743	-3.221	-2.378	Cu_Ag_100_1
-0.565	-1.749	-3.596	-4.037	-1.478	-3.067	-2.317	Cu_Au_100_1
-0.592	-1.782	-3.973	-4.517	-1.798	-3.229	-2.556	Cu_Pd_100_1
-0.609	-1.956	-3.960	-4.590	-1.648	-3.084	-2.692	Cu_Pt_100_1
-1.062	-2.702	-4.510	-5.435	-2.163	-3.221	-3.037	Cu_Ir_100_1
-0.939	-2.328	-4.403	-5.205	-2.116	-3.321	-2.736	Cu_Rh_100_1
-0.741	-1.675	-3.815	-4.712	-1.147	-2.761	-2.718	Pd_Ag_100_1
-0.756	-1.666	-3.691	-4.600	-1.024	-2.635	-2.669	Pd_Au_100_1
-0.758	-1.716	-3.979	-4.800	-1.222	-2.931	-2.754	Pd_Cu_100_1
-0.806	-2.090	-4.108	-4.920	-1.259	-2.742	-2.887	Pd_Pt_100_1
-1.056	-2.759	-4.417	-5.472	-2.034	-3.212	-2.985	Pd_Ir_100_1
-1.035	-2.428	-4.388	-5.382	-1.779	-3.037	-2.834	Pd_Rh_100_1
-1.017	-2.029	-3.890	-4.722	-0.953	-2.677	-2.772	Pt_Ag_100_1
-1.055	-2.047	-3.798	-4.621	-0.853	-2.519	-2.746	Pt_Au_100_1
-1.090	-2.115	-4.015	-4.836	-1.138	-2.983	-2.812	Pt_Cu_100_1
-1.050	-2.076	-3.969	-4.775	-1.127	-2.758	-2.867	Pt_Pd_100_1
-1.281	-2.663	-4.336	-5.274	-1.855	-3.058	-2.942	Pt_Ir_100_1
-1.198	-2.276	-4.078	-5.056	-1.642	-2.972	-2.876	Pt_Rh_100_1
-1.169	-2.914	-4.626	-5.619	-1.854	-3.006	-2.895	Ir_Ag_100_1
-1.226	-2.949	-4.506	-5.470	-1.735	-3.014	-2.860	Ir_Au_100_1
-1.241	-3.184	-4.757	-5.725	-1.961	-3.206	-2.861	Ir_Cu_100_1
-1.233	-3.246	-4.748	-5.677	-1.923	-3.081	-2.894	Ir_Pd_100_1
-1.262	-3.345	-4.598	-5.504	-1.803	-3.062	-2.908	Ir_Pt_100_1
-1.242	-3.453	-4.793	-5.632	-2.068	-3.244	-2.928	Ir_Rh_100_1
-0.965	-2.326	-4.738	-5.825	-2.184	-3.265	-2.750	Rh_Ag_100_1
-0.997	-2.341	-4.610	-5.679	-2.041	-3.149	-2.707	Rh_Au_100_1
-0.708	-2.388	-4.882	-5.944	-2.290	-3.358	-2.787	Rh_Cu_100_1
-0.816	-2.387	-4.894	-5.893	-2.245	-3.322	-2.799	Rh_Pd_100_1
-0.807	-2.103	-4.794	-5.591	-2.093	-3.194	-2.859	Rh_Pt_100_1
-1.033	-2.687	-4.983	-5.879	-2.227	-3.243	-2.925	Rh_Ir_100_1
-0.399	-1.893	-2.325	-2.520	-0.025	-2.072	-2.254	Ag_Au_100_1L
-0.708	-2.993	-4.260	-4.743	-2.193	-3.613	-2.424	Ag_Cu_100_1L
-0.750	-2.674	-4.106	-4.722	-1.323	-2.952	-2.830	Ag_Pd_100_1L
-0.997	-3.424	-4.420	-5.066	-1.688	-3.196	-3.098	Ag_Pt_100_1L
-6.347	-7.318	-8.856	-10.970	-6.312	-7.264	-4.573	Ag_Ir_100_1L
-2.820	-4.623	-5.923	-7.349	-3.510	-4.877	-4.807	Ag_Rh_100_1L
-0.457	-1.532	-2.932	-2.874	-0.844	-3.012	-2.100	Au_Ag_100_1L
-0.794	-2.050	-4.043	-4.362	-1.869	-3.551	-2.401	Au_Cu_100_1L

-0.818	-1.844	-4.009	-4.613	-1.185	-2.964	-2.811	Au_Pd_100_1L
-1.616	-2.301	-4.377	-5.073	-1.684	-3.201	-3.159	Au_Pt_100_1L
-6.375	-7.577	-9.374	-10.029	-6.038	-7.083	-4.302	Au_Ir_100_1L
-2.890	-3.590	-5.322	-6.558	-2.951	-4.072	-4.608	Au_Rh_100_1L
-1.284	-1.855	-2.961	-2.798	-0.563	-2.619	-2.512	Cu_Ag_100_1L
-1.412	-2.029	-2.296	-2.917	-0.502	-2.144	-2.937	Cu_Au_100_1L
-0.553	-2.290	-3.880	-4.580	-1.140	-2.562	-2.605	Cu_Pd_100_1L
-2.190	-2.591	-3.871	-4.011	-1.008	-2.206	-2.663	Cu_Pt_100_1L
-3.023	-3.720	-5.081	-6.029	-2.750	-3.449	-3.196	Cu_Ir_100_1L
-0.941	-3.259	-4.974	-6.019	-2.176	-3.171	-2.748	Cu_Rh_100_1L
-0.396	-1.818	-2.469	-2.321	-0.316	-2.678	-2.013	Pd_Ag_100_1L
-0.428	-1.788	-2.190	-2.388	0.301	-1.863	-2.222	Pd_Au_100_1L
-0.731	-2.733	-3.765	-4.509	-1.506	-3.229	-2.396	Pd_Cu_100_1L
-0.987	-3.154	-3.988	-4.698	-1.297	-2.669	-2.901	Pd_Pt_100_1L
-0.700	-3.864	-5.075	-6.002	-2.527	-3.635	-3.008	Pd_Ir_100_1L
-1.127	-3.494	-4.971	-5.950	-2.301	-3.409	-2.913	Pd_Rh_100_1L
-0.456	-1.892	-2.462	-2.268	-0.268	-2.692	-2.048	Pt_Ag_100_1L
-0.503	-1.884	-2.134	-2.258	0.309	-1.869	-2.297	Pt_Au_100_1L
-0.780	-2.748	-3.573	-4.183	-1.301	-3.257	-2.338	Pt_Cu_100_1L
-0.810	-2.664	-3.853	-4.584	-1.056	-2.867	-2.675	Pt_Pd_100_1L
-1.437	-3.816	-4.919	-5.819	-2.377	-3.520	-3.064	Pt_Ir_100_1L
-1.101	-3.361	-4.748	-5.630	-2.120	-3.326	-2.877	Pt_Rh_100_1L
-0.450	-1.395	-2.642	-2.534	-0.427	-2.697	-2.090	Ir_Ag_100_1L
-0.487	-1.198	-2.319	-2.483	0.227	-1.893	-2.315	Ir_Au_100_1L
-0.711	-1.833	-3.633	-4.615	-1.444	-3.182	-2.347	Ir_Cu_100_1L
-0.744	-1.745	-3.734	-4.396	-1.091	-2.858	-2.623	Ir_Pd_100_1L
-0.922	-1.957	-3.703	-4.327	-0.986	-2.470	-2.824	Ir_Pt_100_1L
-1.017	-2.366	-4.867	-5.763	-2.132	-3.368	-2.849	Ir_Rh_100_1L
-0.381	-1.763	-2.503	-2.474	-0.368	-2.600	-2.041	Rh_Ag_100_1L
-0.380	-1.674	-2.136	-2.433	0.343	-1.761	-2.226	Rh_Au_100_1L
-0.670	-2.650	-3.768	-4.735	-1.594	-3.158	-2.450	Rh_Cu_100_1L
-0.728	-2.517	-3.940	-4.682	-1.243	-2.809	-2.687	Rh_Pd_100_1L
-0.885	-2.870	-3.916	-4.643	-1.057	-2.409	-2.824	Rh_Pt_100_1L
-1.203	-3.546	-4.781	-5.620	-2.193	-3.228	-2.937	Rh_Ir_100_1L
-0.414	-1.947	-2.680	-2.836	-0.633	-2.730	-2.181	Ag_Au_100_2
-0.591	-2.725	-3.593	-3.953	-1.692	-3.423	-2.335	Ag_Cu_100_2
-0.524	-2.418	-3.337	-3.797	-1.091	-2.909	-2.693	Ag_Pd_100_2
-0.534	-2.712	-3.620	-4.493	-1.216	-2.868	-2.925	Ag_Pt_100_2
-0.949	-3.329	-4.831	-6.182	-2.358	-3.666	-3.169	Ag_Ir_100_2
-0.853	-3.263	-4.561	-6.012	-2.304	-3.453	-2.913	Ag_Rh_100_2
-0.594	-2.072	-2.723	-2.771	-0.377	-2.561	-2.354	Au_Ag_100_2
-0.866	-2.647	-3.740	-4.611	-1.236	-3.039	-2.993	Au_Pt_100_2
-0.746	-2.358	-3.166	-3.682	-0.633	-2.857	-2.683	Au_Pd_100_2
-0.866	-2.647	-3.740	-4.611	-1.236	-3.039	-2.993	Au_Pt_100_2

-1.734	-3.331	-4.936	-6.167	-2.348	-3.612	-3.119	Au_Ir_100_2
-1.093	-2.821	-4.595	-5.965	-2.227	-3.487	-2.928	Au_Rh_100_2
-0.576	-2.552	-3.749	-4.142	-1.678	-3.187	-2.381	Cu_Ag_100_2
-0.645	-2.551	-3.492	-3.902	-1.399	-3.088	-2.326	Cu_Au_100_2
-0.629	-2.626	-3.971	-4.504	-1.726	-3.203	-2.592	Cu_Pd_100_2
-0.658	-2.670	-4.002	-4.662	-1.609	-3.138	-2.748	Cu_Pt_100_2
-0.919	-3.215	-4.610	-5.617	-2.126	-3.478	-3.026	Cu_Ir_100_2
-0.856	-3.057	-4.650	-5.625	-2.205	-3.324	-2.743	Cu_Rh_100_2
-0.754	-2.643	-3.848	-4.775	-1.198	-2.903	-2.777	Pd_Ag_100_2
-0.795	-2.661	-3.695	-4.622	-1.036	-2.856	-2.751	Pd_Au_100_2
-0.788	-2.703	-4.002	-4.832	-1.251	-3.102	-2.788	Pd_Cu_100_2
-0.835	-2.966	-4.102	-4.913	-1.394	-2.990	-2.920	Pd_Pt_100_2
-1.137	-3.322	-4.691	-5.737	-2.219	-3.484	-2.980	Pd_Ir_100_2
-1.077	-3.306	-4.596	-5.694	-2.220	-3.409	-2.887	Pd_Rh_100_2
-0.955	-3.085	-3.953	-4.822	-1.332	-3.051	-2.928	Pt_Ag_100_2
-1.024	-3.125	-3.831	-4.682	-1.250	-3.026	-2.918	Pt_Au_100_2
-1.079	-3.157	-4.047	-4.890	-1.405	-3.222	-2.943	Pt_Cu_100_2
-1.021	-3.157	-3.979	-4.798	-1.366	-3.076	-2.918	Pt_Pd_100_2
-1.320	-3.531	-4.640	-5.618	-2.139	-3.440	-3.007	Pt_Ir_100_2
-1.184	-3.359	-4.310	-5.440	-1.973	-3.447	-2.906	Pt_Rh_100_2
-1.100	-2.875	-4.675	-5.701	-2.198	-3.472	-2.990	Ir_Ag_100_2
-1.168	-2.897	-4.535	-5.528	-2.095	-3.466	-2.972	Ir_Au_100_2
-1.173	-3.204	-4.782	-5.767	-2.289	-3.577	-3.014	Ir_Cu_100_2
-1.185	-3.187	-4.738	-5.688	-2.244	-3.524	-2.994	Ir_Pd_100_2
-1.241	-3.329	-4.605	-5.523	-2.162	-3.525	-2.987	Ir_Pt_100_2
-1.214	-3.434	-4.849	-5.697	-2.238	-3.550	-2.984	Ir_Rh_100_2
-0.928	-3.189	-4.795	-5.894	-2.257	-3.472	-2.871	Rh_Ag_100_2
-0.984	-3.227	-4.968	-5.791	-2.130	-3.434	-2.849	Rh_Au_100_2
-0.979	-3.296	-4.910	-5.976	-2.328	-3.554	-2.887	Rh_Cu_100_2
-0.991	-3.268	-4.895	-5.909	-2.265	-3.496	-2.857	Rh_Pd_100_2
-1.042	-3.296	-4.798	-5.599	-2.094	-3.482	-2.877	Rh_Pt_100_2
-1.059	-3.418	-5.006	-5.915	-2.303	-3.560	-2.952	Rh_Ir_100_2
-0.443	-1.870	-2.622	-2.767	-0.539	-2.696	-2.174	Ag_Au_100_4
-0.649	-2.841	-4.123	-4.684	-2.074	-3.532	-2.366	Ag_Cu_100_4
-0.578	-2.435	-3.871	-4.423	-1.279	-2.959	-2.685	Ag_Pd_100_4
-0.633	-2.798	-3.935	-4.698	-1.386	-2.935	-2.850	Ag_Pt_100_4
-0.796	-3.245	-4.711	-5.706	-2.370	-3.635	-3.015	Ag_Ir_100_4
-0.848	-3.200	-4.585	-5.947	-2.295	-3.442	-2.819	Ag_Rh_100_4
-0.559	-2.081	-2.824	-2.788	-0.717	-2.983	-2.365	Au_Ag_100_4
-0.897	-2.762	-4.029	-4.715	-1.595	-3.058	-2.936	Au_Pt_100_4
-0.746	-2.521	-3.792	-4.339	-1.058	-2.901	-2.661	Au_Pd_100_4
-0.897	-2.762	-4.029	-4.715	-1.350	-3.058	-2.936	Au_Pt_100_4
-1.683	-3.261	-4.936	-5.928	-2.499	-3.686	-3.312	Au_Ir_100_4
-1.157	-2.977	-4.834	-6.079	-2.345	-3.589	-2.899	Au_Rh_100_4

-0.425	-2.167	-3.705	-4.064	-1.633	-3.138	-2.409	Cu_Ag_100_4
-0.505	-1.986	-3.529	-3.888	-1.578	-2.995	-2.322	Cu_Au_100_4
-0.558	-2.374	-3.890	-4.433	-1.577	-3.110	-2.589	Cu_Pd_100_4
-0.626	-2.587	-4.027	-4.752	-1.644	-2.878	-2.837	Cu_Pt_100_4
-0.806	-3.147	-5.009	-6.065	-2.474	-3.426	-3.106	Cu_Ir_100_4
-0.864	-3.026	-4.900	-5.901	-2.428	-3.511	-2.987	Cu_Rh_100_4
-0.721	-2.630	-3.962	-4.931	-1.326	-2.906	-2.820	Pd_Ag_100_4
-0.816	-2.634	-3.765	-4.755	-1.104	-2.814	-2.735	Pd_Au_100_4
-0.791	-2.719	-4.092	-4.940	-1.341	-3.195	-2.814	Pd_Cu_100_4
-0.865	-2.998	-4.086	-4.909	-1.318	-2.984	-2.895	Pd_Pt_100_4
-1.284	-3.451	-4.721	-5.701	-2.291	-3.576	-3.024	Pd_Ir_100_4
-1.133	-3.373	-4.915	-5.904	-2.206	-3.492	-2.878	Pd_Rh_100_4
-0.843	-2.557	-4.039	-4.946	-1.407	-2.955	-2.977	Pt_Ag_100_4
-0.950	-2.573	-3.889	-4.784	-1.208	-2.941	-2.937	Pt_Au_100_4
-0.990	-3.039	-4.122	-4.996	-1.539	-3.285	-3.010	Pt_Cu_100_4
-0.969	-2.948	-3.986	-4.813	-1.415	-3.019	-2.925	Pt_Pd_100_4
-1.384	-3.612	-4.714	-5.669	-2.199	-3.517	-3.015	Pt_Ir_100_4
-1.163	-3.354	-4.766	-5.698	-2.045	-3.490	-2.892	Pt_Rh_100_4
-1.055	-3.312	-4.722	-5.787	-2.252	-3.358	-3.099	Ir_Ag_100_4
-1.192	-3.403	-4.567	-5.596	-2.122	-3.431	-3.059	Ir_Au_100_4
-1.087	-3.442	-4.809	-5.844	-2.414	-3.559	-3.116	Ir_Cu_100_4
-1.121	-3.447	-4.712	-5.690	-2.347	-3.527	-3.047	Ir_Pd_100_4
-1.219	-3.501	-4.587	-5.526	-2.182	-3.534	-2.897	Ir_Pt_100_4
-1.165	-3.482	-4.918	-5.828	-2.290	-3.525	-3.004	Ir_Rh_100_4
-0.808	-3.143	-4.821	-5.951	-2.322	-3.370	-2.934	Rh_Ag_100_4
-0.941	-2.279	-4.642	-5.741	-2.108	-3.373	-2.862	Rh_Au_100_4
-0.917	-3.238	-4.910	-6.008	-2.368	-3.531	-2.948	Rh_Cu_100_4
-0.974	-3.268	-4.865	-5.902	-2.267	-3.502	-2.871	Rh_Pd_100_4
-1.054	-3.094	-4.784	-5.761	-2.081	-3.455	-2.865	Rh_Pt_100_4
-1.104	-3.437	-5.046	-5.962	-2.291	-3.572	-2.945	Rh_Ir_100_4
-0.319	-1.546	-2.259	-2.161	-0.165	-2.360	-2.086	Ag_Au_111_1
-0.460	-2.057	-2.881	-2.737	-0.875	-2.973	-2.221	Ag_Cu_111_1
-0.517	-1.890	-2.649	-2.885	-0.520	-2.582	-2.487	Ag_Pd_111_1
-0.515	-2.047	-2.917	-3.407	-0.729	-2.526	-2.753	Ag_Pt_111_1
-1.095	-2.759	-3.922	-5.042	-1.813	-3.198	-3.075	Ag_Ir_111_1
-1.016	-2.493	-3.590	-4.458	-1.484	-3.034	-2.891	Ag_Rh_111_1
-0.462	-1.515	-2.248	-2.212	0.098	-2.106	-2.205	Au_Ag_111_1
-0.656	-1.919	-2.784	-2.761	-0.384	-2.512	-2.263	Au_Cu_111_1
-0.715	-1.829	-2.748	-3.147	-0.233	-2.150	-2.587	Au_Pd_111_1
-0.822	-2.047	-3.027	-3.565	-0.456	-2.405	-2.752	Au_Pt_111_1
-1.320	-2.693	-3.791	-4.814	-1.355	-3.041	-3.045	Au_Ir_111_1
-1.187	-2.375	-3.507	-4.368	-1.030	-2.795	-2.717	Au_Rh_111_1
-0.431	-2.069	-3.404	-3.540	-1.350	-2.967	-2.348	Cu_Ag_111_1
-0.448	-1.786	-3.292	-3.400	-1.247	-2.934	-2.282	Cu_Au_111_1

-0.538	-2.177	-3.393	-3.733	-1.231	-2.840	-2.634	Cu_Pd_111_1
-0.528	-2.212	-3.434	-3.930	-1.198	-2.656	-2.692	Cu_Pt_111_1
-0.930	-2.659	-4.100	-5.012	-1.859	-3.012	-2.913	Cu_Ir_111_1
-0.902	-2.575	-3.986	-4.732	-1.791	-3.057	-2.851	Cu_Rh_111_1
-0.794	-2.489	-3.532	-5.083	-1.072	-2.707	-2.846	Pd_Ag_111_1
-0.802	-1.931	-3.545	-4.281	-0.919	-2.612	-2.771	Pd_Au_111_1
-0.599	-2.317	-4.051	-4.723	-1.518	-2.861	-2.919	Pd_Cu_111_1
-0.925	-2.659	-4.333	-5.167	-1.570	-2.705	-2.969	Pd_Pt_111_1
-1.183	-2.994	-4.726	-5.798	-2.064	-3.110	-2.932	Pd_Ir_111_1
-1.166	-2.949	-4.699	-5.727	-2.038	-3.040	-2.978	Pd_Rh_111_1
-0.869	-2.402	-3.484	-4.336	-0.901	-2.452	-2.759	Pt_Ag_111_1
-0.876	-1.926	-3.503	-4.280	-0.734	-2.320	-2.683	Pt_Au_111_1
-0.933	-2.624	-4.181	-4.993	-1.281	-2.585	-2.801	Pt_Cu_111_1
-0.905	-2.489	-4.098	-4.894	-1.160	-2.464	-2.806	Pt_Pd_111_1
-1.261	-2.785	-4.417	-5.286	-1.572	-2.896	-2.859	Pt_Ir_111_1
-1.137	-2.683	-4.353	-5.216	-1.537	-2.667	-2.817	Pt_Rh_111_1
-0.924	-2.651	-3.829	-4.781	-1.428	-2.771	-2.746	Ir_Ag_111_1
-0.948	-2.622	-3.745	-4.626	-1.222	-2.670	-2.654	Ir_Au_111_1
-0.988	-2.875	-4.149	-4.964	-1.720	-2.918	-2.788	Ir_Cu_111_1
-0.978	-2.786	-4.263	-5.067	-1.668	-2.852	-2.811	Ir_Pd_111_1
-0.971	-2.729	-4.220	-4.990	-1.526	-2.754	-2.706	Ir_Pt_111_1
-0.962	-2.792	-4.514	-5.359	-1.873	-2.863	-2.816	Ir_Rh_111_1
-0.899	-2.760	-3.914	-5.688	-1.596	-3.042	-2.747	Rh_Ag_111_1
-0.931	-2.120	-3.833	-4.785	-2.069	-2.979	-2.842	Rh_Au_111_1
-0.941	-2.926	-4.245	-5.183	-1.903	-3.154	-2.793	Rh_Cu_111_1
-0.711	-2.620	-4.350	-5.285	-1.868	-3.104	-2.842	Rh_Pd_111_1
-0.955	-2.823	-4.347	-5.262	-1.764	-3.025	-2.767	Rh_Pt_111_1
-0.953	-2.872	-4.589	-5.630	-2.032	-3.024	-2.784	Rh_Ir_111_1
-0.293	-1.385	-2.123	-2.291	0.241	-1.882	-2.145	Ag_Au_111_1L
-0.811	-3.041	-4.139	-4.370	-2.234	-3.899	-2.661	Ag_Cu_111_1L
-0.682	-2.314	-4.087	-4.873	-1.487	-2.896	-2.976	Ag_Pd_111_1L
-0.834	-2.667	-4.667	-5.545	-1.731	-2.928	-3.150	Ag_Pt_111_1L
-3.072	-5.799	-6.735	-8.191	-4.051	-5.014	-4.556	Ag_Ir_111_1L
-1.270	-4.079	-6.237	-7.496	-3.516	-4.367	-3.572	Ag_Rh_111_1L
-0.373	-1.698	-2.374	-2.027	-0.285	-2.635	-2.135	Au_Ag_111_1L
-0.937	-3.183	-4.221	-4.131	-2.146	-3.916	-2.751	Au_Cu_111_1L
-0.805	-2.461	-4.125	-4.916	-1.512	-3.012	-2.956	Au_Pd_111_1L
-1.004	-2.738	-4.687	-5.476	-1.698	-2.933	-3.056	Au_Pt_111_1L
-3.088	-6.307	-6.682	-8.497	-3.885	-4.971	-4.638	Au_Ir_111_1L
-1.411	-4.356	-6.164	-7.420	-3.417	-4.293	-3.642	Au_Rh_111_1L
-1.729	-3.744	-3.473	-4.044	-1.624	-3.549	-3.445	Cu_Ag_111_1L
-2.214	-3.316	-3.815	-5.345	-2.062	-3.730	-4.542	Cu_Au_111_1L
-0.406	-1.783	-2.876	-3.581	-0.570	-2.080	-2.582	Cu_Pd_111_1L
-0.353	-1.949	-3.110	-4.116	-0.412	-2.054	-2.721	Cu_Pt_111_1L

-0.492	-2.776	-4.379	-5.101	-1.675	-1.971	-2.684	Cu_Ir_111_1L
-0.624	-2.736	-4.532	-5.373	-1.955	-2.619	-2.722	Cu_Rh_111_1L
-0.341	-1.563	-1.994	-1.855	-0.004	-2.411	-2.005	Pd_Ag_111_1L
-0.294	-1.211	-1.657	-2.021	0.569	-1.770	-1.944	Pd_Au_111_1L
-0.688	-2.522	-3.771	-4.112	-1.711	-3.463	-2.498	Pd_Cu_111_1L
-0.938	-2.500	-4.199	-4.978	-1.251	-2.363	-2.850	Pd_Pt_111_1L
-1.227	-3.344	-5.256	-6.266	-2.388	-3.172	-3.081	Pd_Ir_111_1L
-1.157	-3.426	-5.352	-6.472	-2.682	-3.603	-3.144	Pd_Rh_111_1L
-0.375	-1.640	-2.276	-2.025	-0.184	-2.460	-2.075	Pt_Ag_111_1L
-0.354	-1.322	-1.978	-2.258	0.353	-1.791	-2.056	Pt_Au_111_1L
-0.792	-2.748	-4.044	-4.066	-1.901	-3.686	-2.640	Pt_Cu_111_1L
-0.754	-2.359	-3.896	-4.806	-1.329	-2.675	-2.839	Pt_Pd_111_1L
-1.231	-3.290	-5.177	-6.118	-2.354	-3.205	-3.071	Pt_Ir_111_1L
-1.105	-3.193	-5.114	-6.148	-2.525	-3.511	-2.983	Pt_Rh_111_1L
-0.368	-1.735	-2.417	-2.243	-0.395	-2.531	-2.173	Ir_Ag_111_1L
-0.312	-1.368	-1.951	-2.208	0.239	-1.899	-2.021	Ir_Au_111_1L
-0.713	-2.644	-4.062	-4.115	-1.960	-3.619	-2.586	Ir_Cu_111_1L
-0.696	-2.209	-3.456	-4.195	-1.002	-2.588	-2.703	Ir_Pd_111_1L
-0.707	-1.969	-3.103	-3.866	-0.495	-2.124	-2.534	Ir_Pt_111_1L
-0.948	-2.879	-4.634	-5.561	-2.148	-3.214	-2.894	Ir_Rh_111_1L
-0.301	-1.566	-2.171	-1.991	-0.175	-2.364	-2.061	Rh_Ag_111_1L
-0.223	-1.465	-1.897	-2.013	0.409	-1.746	-1.917	Rh_Au_111_1L
-0.648	-2.585	-4.009	-4.184	-1.914	-3.546	-2.633	Rh_Cu_111_1L
-0.691	-2.196	-3.514	-4.300	-1.040	-2.542	-2.698	Rh_Pd_111_1L
-0.754	-2.093	-3.275	-4.083	-0.575	-2.187	-2.600	Rh_Pt_111_1L
-0.959	-2.736	-4.465	-5.356	-1.732	-2.736	-2.672	Rh_Ir_111_1L
-0.337	-1.592	-2.261	-2.299	-0.151	-2.342	-2.100	Ag_Au_111_2
-0.481	-2.345	-3.411	-3.462	-1.380	-3.248	-2.356	Ag_Cu_111_2
-0.601	-2.250	-3.305	-3.882	-0.994	-2.725	-2.890	Ag_Pd_111_2
-0.595	-2.409	-3.670	-4.533	-1.169	-2.675	-2.990	Ag_Pt_111_2
-0.939	-3.026	-4.693	-6.063	-2.159	-3.354	-3.137	Ag_Ir_111_2
-0.912	-3.082	-4.650	-6.040	-2.283	-3.292	-2.962	Ag_Rh_111_2
-0.450	-1.584	-2.324	-2.292	0.026	-2.314	-2.210	Au_Ag_111_2
-0.686	-2.295	-3.221	-3.146	-0.945	-3.059	-2.353	Au_Cu_111_2
-0.784	-2.248	-3.336	-3.955	-0.760	-2.530	-2.823	Au_Pd_111_2
-0.855	-2.555	-3.749	-4.527	-0.989	-2.525	-2.908	Au_Pt_111_2
-1.229	-3.170	-4.582	-5.847	-1.889	-3.206	-3.062	Au_Ir_111_2
-1.137	-3.109	-4.525	-5.799	-1.925	-3.168	-2.864	Au_Rh_111_2
-0.416	-2.028	-3.364	-3.520	-1.303	-2.893	-2.324	Cu_Ag_111_2
-0.442	-1.748	-3.173	-3.293	-1.128	-2.846	-2.241	Cu_Au_111_2
-0.515	-2.159	-3.419	-3.919	-1.246	-2.830	-2.694	Cu_Pd_111_2
-0.472	-2.209	-3.487	-4.170	-1.108	-2.595	-2.673	Cu_Pt_111_2
-0.828	-2.832	-4.202	-5.265	-1.912	-3.109	-2.989	Cu_Ir_111_2
-0.830	-2.848	-4.273	-5.257	-1.935	-3.080	-2.859	Cu_Rh_111_2

-0.782	-2.467	-3.505	-5.059	-1.067	-2.714	-2.985	Pd_Ag_111_2
-0.789	-2.367	-3.458	-4.211	-0.855	-2.566	-2.757	Pd_Au_111_2
-0.854	-2.621	-4.049	-4.736	-1.548	-2.997	-2.950	Pd_Cu_111_2
-0.928	-2.721	-4.383	-5.212	-1.574	-2.698	-2.992	Pd_Pt_111_2
-1.137	-3.087	-4.851	-5.995	-2.110	-3.117	-2.970	Pd_Ir_111_2
-1.145	-3.205	-4.997	-6.152	-2.336	-3.292	-2.985	Pd_Rh_111_2
-0.860	-2.434	-3.533	-4.378	-1.264	-2.538	-2.771	Pt_Ag_111_2
-0.872	-2.340	-3.511	-4.292	-1.124	-2.349	-2.735	Pt_Au_111_2
-0.986	-2.699	-4.285	-5.099	-1.402	-2.943	-2.845	Pt_Cu_111_2
-0.906	-2.501	-4.160	-4.964	-1.222	-2.496	-2.835	Pt_Pd_111_2
-1.245	-3.036	-4.674	-5.569	-1.848	-2.931	-2.865	Pt_Ir_111_2
-1.138	-2.937	-4.664	-5.587	-1.937	-3.010	-2.883	Pt_Rh_111_2
-0.953	-2.753	-4.582	-5.653	-1.522	-2.860	-2.738	Ir_Ag_111_2
-0.975	-2.681	-4.479	-5.458	-1.815	-2.723	-2.691	Ir_Au_111_2
-1.061	-2.958	-4.321	-5.185	-1.870	-3.018	-2.827	Ir_Cu_111_2
-1.016	-2.856	-4.356	-5.176	-1.765	-2.902	-2.831	Ir_Pd_111_2
-0.993	-2.759	-4.248	-5.024	-1.562	-2.785	-2.702	Ir_Pt_111_2
-0.976	-2.822	-4.586	-5.447	-1.969	-2.954	-2.890	Ir_Rh_111_2
-0.922	-2.805	-4.678	-5.821	-2.175	-3.084	-2.886	Rh_Ag_111_2
-0.948	-2.128	-3.809	-5.623	-2.058	-3.011	-2.852	Rh_Au_111_2
-0.987	-2.966	-4.365	-5.369	-2.020	-3.202	-2.865	Rh_Cu_111_2
-0.955	-2.625	-4.376	-5.262	-1.898	-3.133	-2.863	Rh_Pd_111_2
-0.972	-2.827	-4.319	-5.245	-1.734	-3.028	-2.762	Rh_Pt_111_2
-0.967	-2.900	-4.641	-5.648	-2.073	-3.036	-2.820	Rh_Ir_111_2
-0.349	-1.578	-2.270	-2.394	-0.139	-2.319	-2.120	Ag_Au_111_3
-0.507	-2.442	-3.795	-3.901	-1.764	-3.451	-2.483	Ag_Cu_111_3
-0.587	-2.301	-3.902	-4.708	-1.422	-2.834	-3.003	Ag_Pd_111_3
-0.504	-2.230	-4.115	-5.140	-1.286	-2.715	-2.808	Ag_Pt_111_3
-1.075	-3.033	-5.106	-6.615	-2.475	-3.611	-3.205	Ag_Ir_111_3
-0.991	-3.925	-5.436	-7.062	-2.842	-3.378	-3.032	Ag_Rh_111_3
-0.447	-1.596	-2.324	-2.288	-0.018	-2.536	-2.204	Au_Ag_111_3
-0.750	-2.524	-3.629	-3.583	-1.495	-3.531	-2.470	Au_Cu_111_3
-0.802	-2.366	-3.968	-4.761	-1.317	-2.821	-2.976	Au_Pd_111_3
-0.813	-2.454	-4.336	-5.232	-1.331	-2.462	-2.863	Au_Pt_111_3
-1.354	-3.163	-5.101	-6.496	-2.124	-3.295	-3.134	Au_Ir_111_3
-1.235	-3.183	-5.370	-6.884	-2.667	-3.358	-3.059	Au_Rh_111_3
-0.371	-1.953	-3.300	-3.471	-1.237	-2.820	-2.283	Cu_Ag_111_3
-0.430	-1.866	-2.992	-3.111	-0.957	-2.713	-2.207	Cu_Au_111_3
-0.475	-2.073	-3.397	-4.027	-1.105	-2.879	-2.678	Cu_Pd_111_3
-0.435	-2.011	-3.385	-4.186	-0.942	-2.406	-2.565	Cu_Pt_111_3
-0.891	-2.822	-4.599	-5.693	-2.077	-3.069	-3.022	Cu_Ir_111_3
-0.875	-2.804	-4.699	-5.820	-2.165	-3.073	-2.903	Cu_Rh_111_3
-0.737	-2.437	-3.410	-5.010	-1.514	-2.709	-2.999	Pd_Ag_111_3
-0.751	-2.299	-3.323	-4.107	-1.286	-2.510	-2.727	Pd_Au_111_3

-0.815	-2.623	-4.020	-4.674	-1.535	-3.130	-2.931	Pd_Cu_111_3
-0.926	-2.660	-4.403	-5.218	-1.562	-2.672	-3.007	Pd_Pt_111_3
-1.115	-3.036	-4.865	-6.057	-2.107	-3.108	-2.993	Pd_Ir_111_3
-1.130	-3.146	-5.208	-6.425	-2.496	-3.303	-2.976	Pd_Rh_111_3
-0.878	-2.546	-4.270	-5.107	-1.399	-2.638	-2.876	Pt_Ag_111_3
-0.862	-2.374	-4.056	-4.227	-1.153	-2.379	-2.749	Pt_Au_111_3
-0.930	-2.737	-4.327	-5.151	-1.452	-3.208	-2.851	Pt_Cu_111_3
-0.880	-2.511	-4.223	-5.034	-1.232	-2.515	-2.837	Pt_Pd_111_3
-1.227	-2.989	-4.813	-5.851	-1.986	-2.880	-2.872	Pt_Ir_111_3
-1.141	-3.031	-4.965	-5.989	-2.327	-3.038	-2.946	Pt_Rh_111_3
-1.026	-2.894	-4.854	-5.958	-2.180	-3.000	-2.856	Ir_Ag_111_3
-1.032	-2.774	-4.623	-5.609	-1.963	-2.803	-2.794	Ir_Au_111_3
-1.157	-3.109	-4.927	-6.064	-2.247	-3.166	-2.921	Ir_Cu_111_3
-1.015	-2.902	-4.273	-5.118	-2.099	-2.945	-2.822	Ir_Pd_111_3
-1.006	-2.777	-4.141	-4.951	-1.887	-2.807	-2.679	Ir_Pt_111_3
-0.977	-2.841	-4.620	-5.475	-2.040	-3.070	-2.926	Ir_Rh_111_3
-0.881	-2.851	-4.808	-5.920	-2.302	-3.134	-2.925	Rh_Ag_111_3
-0.932	-2.710	-4.611	-5.621	-2.083	-3.007	-2.867	Rh_Au_111_3
-0.985	-2.993	-4.384	-6.097	-2.058	-3.253	-2.850	Rh_Cu_111_3
-0.951	-2.880	-4.314	-5.671	-1.836	-3.168	-2.807	Rh_Pd_111_3
-0.984	-2.833	-4.282	-5.229	-1.968	-3.037	-2.756	Rh_Pt_111_3
-0.969	-2.912	-4.691	-5.665	-2.113	-3.046	-2.828	Rh_Ir_111_3
-1.270	-3.560	-4.710	-5.480	-2.150	-3.540	-2.970	Ir_100
-0.600	-2.630	-4.110	-4.700	-2.000	-3.350	-2.430	Cu_100
-0.790	-2.710	-4.090	-5.070	-1.200	-2.760	-2.770	Pd_100
-1.090	-3.200	-3.830	-4.610	-1.310	-3.070	-2.910	Pt_100
-1.020	-3.300	-5.040	-5.890	-2.280	-3.370	-2.850	Rh_100
-0.380	-1.980	-2.820	-2.920	-0.870	-2.930	-1.980	Ag_100
-0.500	-2.110	-2.460	-2.550	-0.020	-2.210	-2.330	Au_100
-0.300	-1.640	-2.240	-1.960	-0.250	-2.590	-2.060	Ag_111
-0.330	-1.480	-2.280	-2.370	0.190	-1.890	-2.180	Au_111
-0.950	-2.710	-4.440	-5.300	-1.750	-2.730	-2.710	Ir_111
-0.480	-2.190	-3.420	-3.540	-1.380	-3.030	-2.480	Cu_111
-0.830	-2.540	-4.240	-5.050	-1.550	-2.750	-2.970	Pd_111
-0.890	-2.410	-4.020	-4.810	-1.120	-2.350	-2.730	Pt_111
-0.970	-2.900	-4.640	-5.670	-2.130	-3.140	-2.850	Rh_111

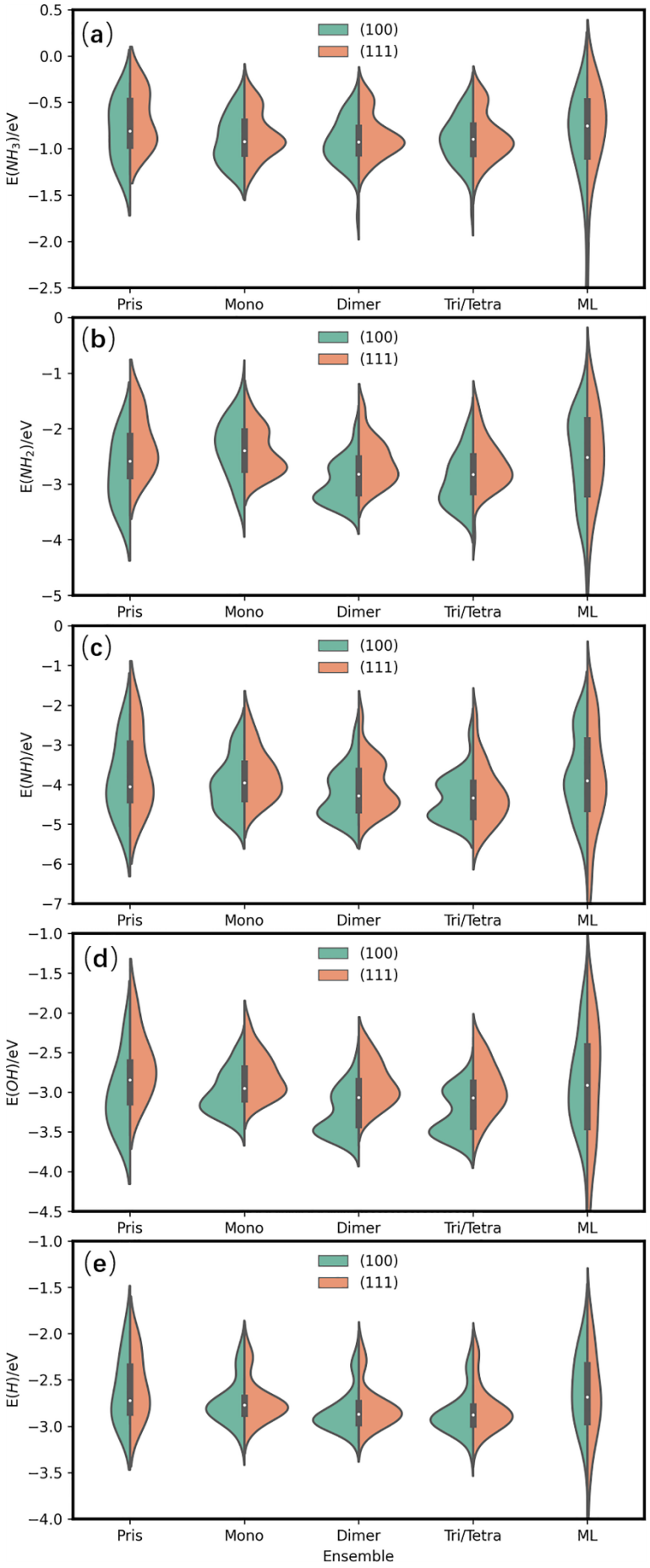
(a)
(b)
(c)
(d)
(e)
(100)
(111)
E(NH3)/eV
E(NH2)/eV
E(NH)/eV
E(OH)/eV
E(H)/eV
Pris
Mono
Dimer
Tri/Tetra
ML
Ensemble

Fig. S3. The violin plots of E(N) and E(O) on different ensembles of (100) and (111) (Pris: pristine systems; Mono: monomer; Dimer: dimer; Tri: trimer; Tetra: tetramer; ML: monolayer).

Table S6. The predictive performance of 1st and 2nd K-means analysis.

Model	Number of clusters	Data type	Silhouette score	Calinski harabasz score
1st K-means	3	train	0.52	647.62
		test	0.49	121.40
2nd K-means	3	train	0.45	98.07
		test	0.37	21.85

Table S7. Three clusters of 1st clustering analysis on catalytic performance.

C_{11}			C_{12}			C_{13}		
-1.44975	0.020584	Center	2.955782	0.111276	Center	0.229632	-0.00847	Center
-1.78224	0.11796	Ir_Rh_100_1	2.279763	0.547182	Au_Ag_100_1L	1.223694	0.48595	Cu_Ag_111_1
-0.75286	-0.43313	Pd_Pt_111_2	3.161614	0.411886	Ir_Ag_111_1L	-0.02343	-0.36183	Pt_Cu_100_1
-1.48079	-0.18545	Cu_Ir_111_3	3.412524	0.014034	Au_Ag_111_2	0.412309	-0.03963	Au_Pd_100_4
-0.85983	-0.13322	Ir_Pd_111_2	2.5849	0.104306	Au_Ag_100_1	-0.08766	1.036574	Pt_Cu_111_1L
-1.37753	-0.19892	Rh_Au_111_3	4.17748	-0.34715	Rh_Au_111_1L	0.440167	-0.38606	Pt_Au_111_3
-1.0644	-0.22487	Ir_Rh_111_1	2.542515	0.139231	Au_Cu_111_1	0.394689	0.871304	Ag_Cu_111_3
-1.95484	0.369606	Pt_Ir_100_4	2.204513	0.635585	Ag_100	-0.50729	-0.3605	Pd_111
-1.18791	0.114321	Rh_Cu_111_2	3.591309	-0.13556	Au_Ag_111_1	0.091984	-0.26454	Pd_Au_100_4
-0.87238	-0.33929	Ir_111	3.882306	0.36107	Pd_Ag_111_1L	0.233847	0.765854	Pd_Cu_111_1L
-0.81361	0.314899	Ag_Ir_100_1	2.436073	0.40163	Ag_Au_100_2	-0.58881	-0.26009	Pt_Cu_111_2
-1.9498	0.184436	Rh_Ag_100_2	3.195895	-0.16048	Ag_Au_100_1L	0.006255	-0.3889	Pt_Pd_111_1L
-0.94545	0.033125	Rh_Pt_111_3	3.552027	-0.39526	Pd_Au_100_1L	0.345905	-0.40377	Cu_Pd_100_1L
-1.47722	0.192546	Ir_Au_100_2	3.543563	-0.58008	Ir_Au_100_1L	0.056381	-0.20445	Rh_Pd_100_1L
-1.38765	-0.25869	Ir_Ag_100_1	3.643898	0.317417	Rh_Ag_111_1L	0.156117	0.272205	Ag_Rh_100_1
-1.96843	0.393214	Pd_Ir_100_4	3.390938	0.136375	Ag_Au_111_2	-0.2162	0.218793	Cu_Pt_100_2
-1.82094	-0.29374	Ir_Ag_111_3	3.617624	-0.31903	Pt_Au_100_1L	0.463627	-0.6904	Pt_Au_100_1
-1.80718	0.231731	Pt_Rh_100_4	4.407026	-0.46551	Pd_Au_111_1L	-0.23671	0.121496	Pd_Cu_111_3
-1.92838	-0.23272	Pd_Ir_111_2	2.573993	0.353652	Ag_Au_100_4	1.297605	-0.68832	Rh_Pt_111_1L
-1.21389	-0.42291	Ag_Pt_111_1L	3.769671	-0.39607	Ag_Au_111_1L	-0.45342	-0.0594	Pd_Pt_100_2
-1.42759	-0.11423	Rh_Au_100_4	2.061502	0.484938	Au_Cu_100_1	0.385653	-0.52349	Pd_Ag_100_1
-2.1994	0.18634	Pd_Rh_100_1L	1.986689	-0.55861	Cu_Pd_111_1L	0.052977	-0.02592	Au_Pt_100_2
-1.41923	-0.19773	Pt_Rh_111_2	3.493002	0.212035	Ag_Au_111_1	0.346378	-0.45552	Au_Pt_111_2
-2.04497	0.211164	Rh_Pd_100_2	2.237004	0.161219	Cu_Ag_100_1L	0.418729	0.377759	Cu_Ag_100_1
-1.88233	0.439522	Ag_Ir_100_4	2.458241	-0.23919	Cu_Au_100_1L	0.315797	0.583225	Cu_Ag_100_2
-1.75145	0.255079	Pd_Rh_100_2	2.22912	0.622624	Au_Ag_100_4	1.469886	-0.04643	Au_Pt_100_1
-1.28814	-0.22186	Rh_Pt_100_1	1.917985	0.237309	Ag_Pd_100_1	-0.23769	-0.09906	Au_Ir_111_1
-1.25552	-0.00771	Pd_Ir_100_1	3.514852	0.378027	Pt_Ag_111_1L	-0.01673	-0.17935	Pd_Ag_100_2
-2.04166	0.212258	Cu_Rh_100_4	1.995159	0.345986	Cu_Au_111_3	0.837391	-0.20082	Cu_Pt_111_2

-1.32051	0.039658	Cu_Ir_100_1	2.216994	0.727008	Ag_Cu_111_1	-0.36139	0.034359	Pt_Ag_100_2
-0.69203	0.254128	Au_Ir_100_1	2.507407	0.199831	Au_Ag_100_2	0.430905	0.513669	Pt_Cu_100_1L
-0.79445	-0.1582	Au_Pt_100_1L	3.366032	0.54015	Au_Ag_111_1L	-0.11502	0.407205	Cu_Pd_100_2
-1.98612	0.095996	Rh_Ag_100_4	3.947403	-0.48684	Pt_Au_111_1L	0.853372	0.40266	Cu_Au_100_4
-1.52759	-0.05953	Rh_111	3.351734	0.192407	Au_Ag_111_3	0.723213	0.98735	Au_Cu_111_3
-1.72249	0.450597	Ir_Pt_100_4	1.720831	0.371425	Cu_Au_111_2	0.830306	-0.14488	Pd_Au_111_3
-1.6993	-0.13302	Rh_Pd_100_1	3.924108	-0.31717	Ir_Au_111_1L	0.601604	-0.59547	Pd_Au_100_1
-0.77326	0.878836	Ag_Cu_100_1L	2.448793	0.156053	Ag_Pd_111_1	-0.05895	0.855538	Rh_Cu_111_1L
-0.909	-0.08402	Rh_Pt_111_1	1.747593	-0.36513	Au_Pt_111_1	1.129258	0.549111	Cu_111
-1.76986	0.130458	Rh_Pt_100_4	2.997349	-0.04938	Au_100	1.509493	0.426318	Cu_Au_111_1
-1.01305	-0.40165	Ir_Au_111_2	2.973876	0.360875	Rh_Ag_100_1L	-0.23595	-0.02727	Cu_Pt_100_4
-1.65555	0.26005	Cu_Ir_100_2	3.535768	0.536351	Ag_111	0.014937	-0.22697	Ag_Pd_111_3
-1.90741	0.14729	Ir_Ag_100_4	2.627026	0.239901	Ag_Au_100_1	-0.48341	-0.24891	Ir_Pt_111_1
-2.29931	0.406091	Pt_Ir_100_1L	2.91676	0.30056	Ir_Ag_100_1L	1.448378	0.056887	Ag_Pt_100_1
-1.04933	0.199185	Ag_Pt_100_1L	3.103742	0.514145	Pt_Ag_100_1L	-0.33295	-0.21331	Pt_Ag_100_4
-1.39392	-0.15387	Rh_Ir_111_1	3.332026	0.061097	Ag_Au_111_3	0.262951	0.030234	Ag_Pd_100_4
-0.9213	0.133164	Rh_Cu_111_1	2.402808	-0.44171	Au_Pd_111_1	0.534485	-0.45634	Cu_Pt_100_1L
-1.59189	-0.11096	Ir_Rh_100_1L	3.624041	-0.53094	Rh_Au_100_1L	-0.32508	-0.4174	Pd_100
-0.94965	0.015248	Ir_Cu_111_2	2.276361	-0.04369	Au_Pd_100_1	1.403875	0.662451	Ag_Cu_100_1
-0.72016	-0.07079	Pt_Cu_111_3	3.581864	-0.39913	Au_111	-0.05121	-0.30034	Au_Pd_111_3
-0.99087	-0.34589	Cu_Rh_111_1L	1.616425	0.62677	Au_Cu_111_2	0.693949	-0.55072	Ir_Pt_100_1L
-1.68711	-0.05877	Ir_Cu_100_1	1.813355	-0.06502	Ag_Pt_111_1	0.100794	0.223938	Cu_Pd_100_1
-1.6889	0.142699	Ir_Ag_100_2	3.08377	0.487824	Pd_Ag_100_1L	1.445651	0.359324	Cu_Ag_111_3
-1.97972	0.352967	Ir_Rh_100_2				-0.48513	-0.74518	Cu_Ir_111_1L
-1.40164	-0.25778	Pt_Ir_111_2				0.225549	-0.18958	Pd_Au_100_2
-1.83908	0.192641	Rh_Ir_100_1L				-0.55462	0.154327	Pt_Cu_100_2
-1.68131	-0.17397	Au_Ir_111_2				0.941548	0.124899	Cu_Pd_111_2
-1.42975	-0.07287	Ir_Pt_100_1				0.830758	-0.4394	Pd_Au_111_1
-0.66526	-0.1638	Ir_Pd_111_1				1.031233	0.249542	Ag_Pd_100_2
-1.68617	-0.39277	Pt_Ir_111_3				1.058801	-0.43659	Cu_Pt_111_3
-1.92031	0.15405	Rh_Au_100_2				0.047356	0.400224	Pd_Cu_100_1L
-1.53867	-0.17285	Rh_Ag_100_1				-0.37051	-0.14149	Au_Pd_111_1L
-1.82723	-0.14341	Rh_Ag_111_3				-0.10185	0.250715	Rh_Cu_100_1L
-1.19759	-0.21159	Ir_Au_100_1				-0.33114	0.109335	Au_Pt_100_4
-2.36898	0.307885	Au_Ir_100_4				-0.00341	0.634811	Au_Cu_100_1L
-1.81265	0.30328	Pt_Ir_100_2				-0.42114	-0.08129	Pd_Pt_100_4
-0.60344	1.247798	Ag_Cu_111_1L				-0.21234	-0.04422	Pd_Cu_100_2
-1.38713	0.323016	Pt_Rh_100_2				1.115858	0.801839	Ag_Cu_111_2
-0.95441	0.031953	Cu_Rh_111_2				0.348619	0.029902	Au_Rh_100_1
-1.69054	-0.17606	Pd_Ir_111_1				1.128718	-0.31263	Au_Pd_111_2
-2.13657	0.352478	Ir_Cu_100_4				-0.47218	-0.24011	Pt_Rh_100_1
-1.86665	0.264616	Pd_Ir_100_2				-0.22824	-0.71364	Pd_Pt_111_1L
-0.95399	-0.02598	Rh_Pd_111_2				-0.09865	-0.17818	Ir_Ag_111_1
-0.93726	0.016569	Cu_Ir_111_2				0.810599	0.265893	Cu_Au_100_1

-0.74048	-0.47964	Pd_Pt_111_3
-1.52329	-0.12538	Rh_Ir_111_3
-1.5551	0.280727	Cu_Au_111_1L
-2.14472	0.247899	Rh_Cu_100_2
-0.92147	-0.25538	Pd_Rh_100_1
-0.66053	0.110793	Ag_Ir_111_1
-1.77404	0.456309	Ir_100
-1.19463	-0.37603	Au_Pt_111_1L
-2.25604	0.264321	Rh_Ir_100_4
-2.08001	0.201568	Pd_Rh_100_4
-1.30827	-0.3613	Ir_Au_111_3
-1.87918	0.184438	Ag_Rh_100_4
-1.59756	-0.21871	Pd_Rh_111_1
-1.73667	-0.10414	Rh_Cu_100_1
-0.6766	-0.41815	Pd_Pt_111_1
-1.81536	0.039338	Au_Rh_100_2
-1.94999	0.393641	Ir_Pd_100_4
-1.84653	-0.14575	Rh_Ir_100_1
-1.73868	0.286271	Rh_Pt_100_2
-1.62364	-0.19696	Cu_Rh_111_3
-1.70756	0.268658	Ir_Au_100_4
-0.9187	-0.35817	Rh_Ir_111_1L
-1.2457	-0.14053	Rh_Pd_111_3
-0.81633	-0.31549	Rh_Au_111_2
-1.47126	0.040083	Ir_Rh_111_1L
-2.19748	0.28256	Rh_Ir_100_2
-1.30234	-0.22512	Rh_Au_100_1
-0.97822	-0.12177	Pt_Ir_100_1
-0.63067	0.014538	Cu_Ir_111_1
-1.12698	-0.51764	Ir_Ag_111_2
-1.58315	0.188782	Cu_Rh_100_2
-0.87559	-0.08366	Rh_Pt_111_2
-2.02785	0.220096	Rh_Pd_100_4
-2.09482	0.138527	Rh_100
-2.12656	0.3029	Ir_Rh_100_4
-1.84297	0.280711	Ir_Pd_100_2
-1.68521	0.371988	Ir_Pt_100_2
-1.46512	-0.13957	Rh_Ir_111_2
-1.95154	0.297428	Ir_Cu_100_2
-0.94404	0.161846	Cu_Rh_100_1
-1.74253	0.192132	Pt_Rh_100_1L
-0.6906	0.159723	Pt_Cu_100_4
-0.71064	-0.46346	Pt_Rh_111_1
-0.90003	-0.31475	Pt_Ir_111_1
-0.20851	-0.61993	Pt_Pd_111_2
-0.19166	0.066427	Pt_Au_100_2
0.072554	0.05022	Cu_Pt_100_1
0.168673	0.124066	Ag_Rh_111_1
-0.35912	0.011161	Pt_Pd_100_4
0.28776	-0.60079	Pt_Ag_100_1
0.632008	-0.28728	Ir_Pd_100_1L
0.34913	0.059628	Ir_Cu_100_1L
0.715543	-0.45178	Pt_Ag_111_1
0.68435	-0.42286	Pt_Au_111_2
-0.52351	1.348645	Au_Cu_111_1L
1.372627	0.058838	Au_Pd_100_2
-0.09303	-0.62877	Pt_Pd_111_1
1.307237	0.420885	Cu_Ag_111_2
-0.33305	0.148185	Cu_Rh_111_1
0.174252	-0.15256	Pt_Pd_100_1L
-0.10331	-0.16669	Pd_Cu_111_1
0.535605	-0.19689	Au_Rh_111_1
-0.235	-0.56959	Ag_Pt_111_3
0.166618	-0.24845	Ir_Au_111_1
-0.20564	0.174952	Pt_100
0.963408	-0.00758	Cu_Pt_111_1
-0.54341	0.781383	Ag_Cu_100_4
0.745932	-0.35151	Rh_Pd_111_1L
-0.55117	-0.22286	Ir_Pt_111_2
0.046502	-0.5526	Pd_Ag_111_1
-0.48608	-0.75007	Au_Pt_111_3
-0.27857	-0.0028	Pd_Cu_111_2
0.13333	0.25469	Cu_Pd_100_4
-0.60019	-0.01142	Ir_Cu_111_1
-0.42339	0.551276	Cu_100
-0.23282	0.006181	Au_Pt_100_4
0.100817	-0.474	Rh_Pt_100_1L
-0.20618	0.954401	Cu_Ag_111_1L
1.082883	0.230547	Cu_Pd_111_1
-0.02478	-0.35913	Pd_Ag_111_3
-0.39071	########	Pd_Cu_100_4
-0.58984	-0.02067	Ir_Pt_111_3
-0.22533	-0.21477	Pd_Ag_100_4
-0.12896	-0.00884	Ag_Pt_100_4
0.229957	-0.30577	Au_Pd_100_1L
0.491588	-0.25554	Pt_Ag_111_2
-0.09074	-0.52637	Pd_Pt_100_1
0.052977	-0.02592	Au_Pt_100_2

-2.03053	-0.21204	Pt_Rh_111_3				1.621743	-0.6702	Ir_Pt_111_1L
-1.56856	-0.13586	Au_Rh_111_2				0.72904	0.534381	Cu_Au_100_2
-1.62453	-0.18395	Rh_Ag_111_2				0.266406	-0.03831	Ag_Pt_100_2
-0.90166	-0.05111	Rh_Pd_111_1				0.84457	-0.27898	Ir_Pd_111_1L
-1.63323	-0.12543	Ir_Pd_100_1				0.828864	-0.33502	Pd_Au_111_2
-0.93616	0.084714	Ir_Pd_111_3				-0.26023	0.069545	Rh_Au_111_1
-0.89418	-0.33092	Rh_Ag_111_1				-0.08989	0.975566	Ir_Cu_111_1L
-1.33316	-0.0803	Ir_Rh_111_3				-0.18053	-0.08416	Ag_Pd_100_1L
-1.2358	-0.17374	Ir_Rh_111_2				0.546149	0.468645	Cu_Ag_100_4
						1.073902	-0.04202	Ag_Pd_111_2
						0.062926	-0.56562	Pd_Ag_111_2
						0.960073	0.030149	Cu_Pd_111_3
						-0.22677	-0.16512	Pd_Pt_100_1L
						-0.23401	-0.24567	Ag_Pd_111_1L
						0.075496	-0.68692	Pt_111
						-0.47096	-0.51607	Pt_Ag_111_3
						0.096279	-0.50734	Pt_Pd_100_1
						-0.08389	-0.21434	Pt_Au_100_4
						-0.31375	-0.51072	Pt_Cu_111_1
						0.41819	0.908041	Ag_Cu_100_2
						0.343912	-0.31254	Ag_Pt_111_2
						1.523707	-0.89034	Cu_Pt_111_1L
						0.987871	-0.70674	Pt_Au_111_1
						-0.2927	-0.63636	Pt_Pd_111_3
						0.165548	-0.42319	Pd_Cu_100_1
						-0.40491	0.093468	Pt_Pd_100_2

Table S8. Three clusters of 2nd clustering analysis on catalytic performance.

C_{21}			C_{22}			C_{23}		
-0.1131	-0.21198	Center	0.149029	0.668409	Center	1.028499	-0.12655	Center
-0.01673	-0.17935	Pd_Ag_100_2	0.723213	0.98735	Au_Cu_111_3	0.941548	0.124899	Cu_Pd_111_2
-0.19166	0.066427	Pt_Au_100_2	0.546149	0.468645	Cu_Ag_100_4	0.830306	-0.14488	Pd_Au_111_3
-0.50729	-0.3605	Pd_111	0.315797	0.583225	Cu_Ag_100_2	1.621743	-0.6702	Ir_Pt_111_1L
-0.23769	-0.09906	Au_Ir_111_1	-0.05895	0.855538	Rh_Cu_111_1L	1.523707	-0.89034	Cu_Pt_111_1L
0.346378	-0.45552	Au_Pt_111_2	-0.52351	1.348645	Au_Cu_111_1L	1.129258	0.549111	Cu_111
-0.10331	-0.16669	Pd_Cu_111_1	0.418729	0.377759	Cu_Ag_100_1	1.448378	0.056887	Ag_Pt_100_1
-0.12896	-0.00884	Ag_Pt_100_4	0.394689	0.871304	Ag_Cu_111_3	0.960073	0.030149	Cu_Pd_111_3
-0.55117	-0.22286	Ir_Pt_111_2	-0.08766	1.036574	Pt_Cu_111_1L	1.058801	-0.43659	Cu_Pt_111_3
-0.09303	-0.62877	Pt_Pd_111_1	-0.20618	0.954401	Cu_Ag_111_1L	1.223694	0.48595	Cu_Ag_111_1
-0.09865	-0.17818	Ir_Ag_111_1	-0.11502	0.407205	Cu_Pd_100_2	1.445651	0.359324	Cu_Ag_111_3
-0.48513	-0.74518	Cu_Ir_111_1L	0.41819	0.908041	Ag_Cu_100_2	0.68435	-0.42286	Pt_Au_111_2
-0.60019	-0.01142	Ir_Cu_111_1	0.100794	0.223938	Cu_Pd_100_1	1.297605	-0.68832	Rh_Pt_111_1L
0.056381	-0.20445	Rh_Pd_100_1L	0.72904	0.534381	Cu_Au_100_2	0.534485	-0.45634	Cu_Pt_100_1L

-0.32508	-0.4174	Pd_100	0.13333	0.25469	Cu_Pd_100_4	0.693949	-0.55072	Ir_Pt_100_1L
0.052977	-0.02592	Au_Pt_100_2	0.156117	0.272205	Ag_Rh_100_1	1.031233	0.249542	Ag_Pd_100_2
-0.33295	-0.21331	Pt_Ag_100_4	0.047356	0.400224	Pd_Cu_100_1L	0.84457	-0.27898	Ir_Pd_111_1L
-0.35912	0.011161	Pt_Pd_100_4	-0.54341	0.781383	Ag_Cu_100_4	0.828864	-0.33502	Pd_Au_111_2
-0.22677	-0.16512	Pd_Pt_100_1L	0.233847	0.765854	Pd_Cu_111_1L	0.715543	-0.45178	Pt_Ag_111_1
0.262951	0.030234	Ag_Pd_100_4	-0.08989	0.975566	Ir_Cu_111_1L	0.810599	0.265893	Cu_Au_100_1
0.225549	-0.18958	Pd_Au_100_2	-0.42339	0.551276	Cu_100	0.830758	-0.4394	Pd_Au_111_1
-0.235	-0.56959	Ag_Pt_111_3	-0.00341	0.634811	Au_Cu_100_1L	1.115858	0.801839	Ag_Cu_111_2
0.096279	-0.50734	Pt_Pd_100_1	0.430905	0.513669	Pt_Cu_100_1L	1.372627	0.058838	Au_Pd_100_2
0.006255	-0.3889	Pt_Pd_111_1L				0.853372	0.40266	Cu_Au_100_4
0.266406	-0.03831	Ag_Pt_100_2				0.837391	-0.20082	Cu_Pt_111_2
0.28776	-0.60079	Pt_Ag_100_1				0.963408	-0.00758	Cu_Pt_111_1
-0.27857	-0.0028	Pd_Cu_111_2				0.601604	-0.59547	Pd_Au_100_1
-0.47218	-0.24011	Pt_Rh_100_1				1.128718	-0.31263	Au_Pd_111_2
0.343912	-0.31254	Ag_Pt_111_2				1.469886	-0.04643	Au_Pt_100_1
-0.22533	-0.21477	Pd_Ag_100_4				1.403875	0.662451	Ag_Cu_100_1
-0.09074	-0.52637	Pd_Pt_100_1				1.307237	0.420885	Cu_Ag_111_2
-0.20851	-0.61993	Pt_Pd_111_2				1.509493	0.426318	Cu_Au_111_1
0.072554	0.05022	Cu_Pt_100_1				0.987871	-0.70674	Pt_Au_111_1
0.046502	-0.5526	Pd_Ag_111_1				0.535605	-0.19689	Au_Rh_111_1
0.075496	-0.68692	Pt_111				1.073902	-0.04202	Ag_Pd_111_2
-0.20564	0.174952	Pt_100				0.745932	-0.35151	Rh_Pd_111_1L
-0.21234	-0.04422	Pd_Cu_100_2				1.082883	0.230547	Cu_Pd_111_1
-0.45342	-0.0594	Pd_Pt_100_2				0.491588	-0.25554	Pt_Ag_111_2
-0.23595	-0.02727	Cu_Pt_100_4				0.632008	-0.28728	Ir_Pd_100_1L
0.014937	-0.22697	Ag_Pd_111_3						
-0.08389	-0.21434	Pt_Au_100_4						
-0.42114	-0.08129	Pd_Pt_100_4						
0.385653	-0.52349	Pd_Ag_100_1						
-0.47096	-0.51607	Pt_Ag_111_3						
-0.33114	0.109335	Au_Pt_100_4						
-0.05121	-0.30034	Au_Pd_111_3						
0.091984	-0.26454	Pd_Au_100_4						
-0.2927	-0.63636	Pt_Pd_111_3						
-0.37051	-0.14149	Au_Pd_111_1L						
0.166618	-0.24845	Ir_Au_111_1						
-0.02343	-0.36183	Pt_Cu_100_1						
0.440167	-0.38606	Pt_Au_111_3						
-0.39071	########	Pd_Cu_100_4						
0.412309	-0.03963	Au_Pd_100_4						
-0.33305	0.148185	Cu_Rh_111_1						
-0.58881	-0.26009	Pt_Cu_111_2						
-0.18053	-0.08416	Ag_Pd_100_1L						
-0.23671	0.121496	Pd_Cu_111_3						

-0.10185	0.250715	Rh_Cu_100_1L
-0.02478	-0.35913	Pd_Ag_111_3
0.165548	-0.42319	Pd_Cu_100_1
-0.2162	0.218793	Cu_Pt_100_2
0.348619	0.029902	Au_Rh_100_1
-0.55462	0.154327	Pt_Cu_100_2
-0.48608	-0.75007	Au_Pt_111_3
0.34913	0.059628	Ir_Cu_100_1L
0.174252	-0.15256	Pt_Pd_100_1L
-0.23282	0.006181	Au_Pt_100_4
-0.26023	0.069545	Rh_Au_111_1
0.052977	-0.02592	Au_Pt_100_2
-0.58984	-0.02067	Ir_Pt_111_3
0.100817	-0.474	Rh_Pt_100_1L
-0.40491	0.093468	Pt_Pd_100_2
0.463627	-0.6904	Pt_Au_100_1
0.062926	-0.56562	Pd_Ag_111_2
0.229957	-0.30577	Au_Pd_100_1L
-0.36139	0.034359	Pt_Ag_100_2
-0.22824	-0.71364	Pd_Pt_111_1L
0.168673	0.124066	Ag_Rh_111_1
-0.23401	-0.24567	Ag_Pd_111_1L
-0.31375	-0.51072	Pt_Cu_111_1
-0.48341	-0.24891	Ir_Pt_111_1
0.345905	-0.40377	Cu_Pd_100_1L

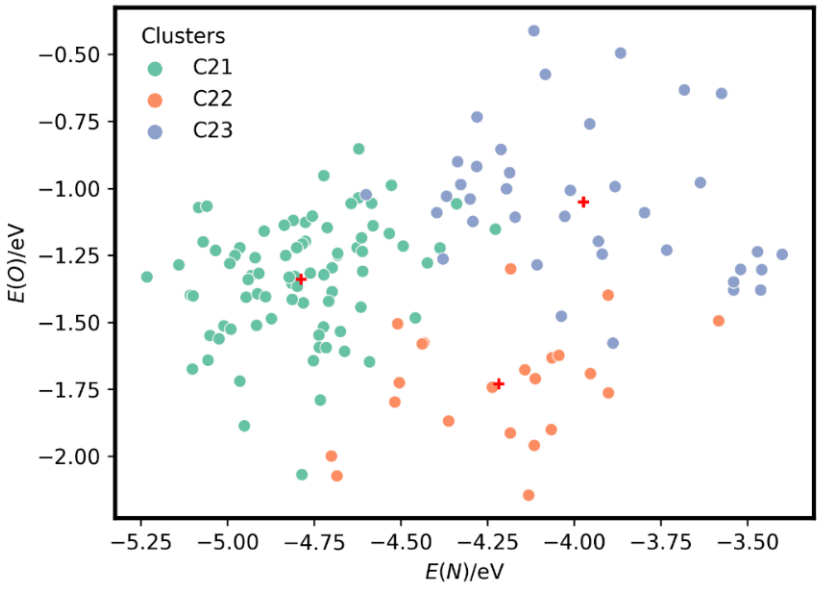

Fig. S4. The distribution of N and O binding energy (E(N) and E(O)) on ensembles in C_{21}, C_{22} and C_{23} clusters. The average E(N) and E(O) of every cluster are denoted with the plus ("+").

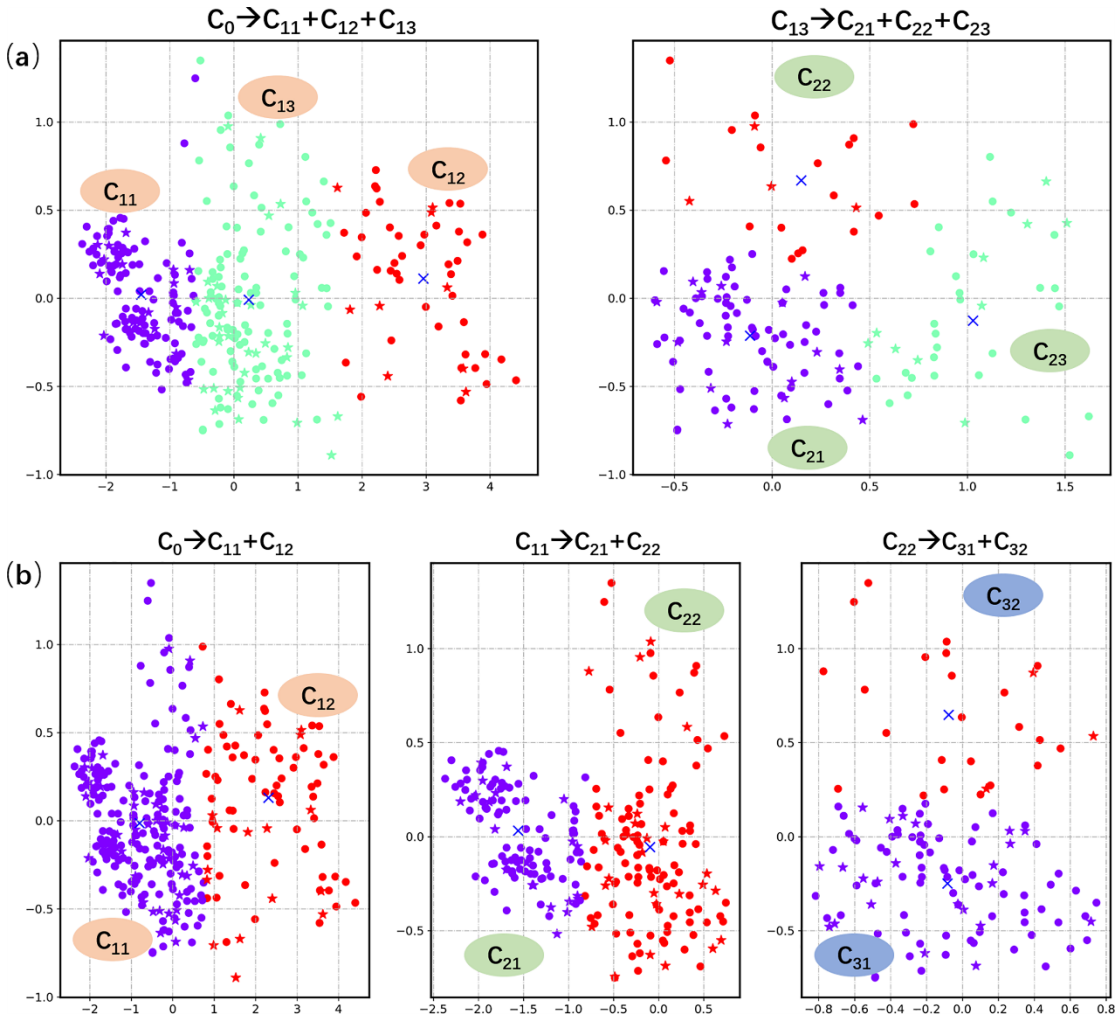

Fig. S5. Different clustering models:(a) twice K-means clustering with 3 and 3 clusters, respectively (K-means-33); (b) three times K-means clustering with 2, 2 and 2 clusters, respectively (K-means-222).

Table S9. The performance of different K-means based clustering models (K-means-33, and K-means-222).

Clustering Model	Numbers	Data types	Silhouette score	Calinski harabasz score
K-means-33	3	train/test	0.52/0.49	647.62/121.40
	3	train/test	0.45/0.37	98.07/21.85
K-means-222	2	train/test	0.59/0.54	497.63/94.91
	2	train/test	0.55/0.47	361.07/64.97
	2	train/test	0.41/0.40	63.52/11.62

Table S10. The detailed systems of C_{21} and C_{31} as well as C_{22} and C_{32} for K-means-33 and K-means-222 clustering models, respectively.

Clustering-33	**Clustering-222**	**K-means-33**	**K-means-222**
C_{21}	**C_{31}**	**C_{22}**	**C_{32}**
Pd_Ag_100_2	Pd_Ag_100_2	Pd_Cu_111_1L	Pd_Cu_111_1L
Pt_Au_100_2	Pt_Au_100_2	Cu_100	Cu_100
Pd_111	Pd_111	Rh_Cu_111_1L	Rh_Cu_111_1L
Au_Ir_111_1	Au_Ir_111_1	Au_Cu_111_1L	Au_Cu_111_1L
Au_Pt_111_2	Au_Pt_111_2	Ag_Cu_100_4	Ag_Cu_100_4
Pd_Cu_111_1	Pd_Cu_111_1	Au_Cu_100_1L	Au_Cu_100_1L
Ag_Pt_100_4	Ag_Pt_100_4	Ir_Cu_111_1L	Ir_Cu_111_1L
Ir_Pt_111_2	Ir_Pt_111_2	Cu_Ag_111_1L	Cu_Ag_111_1L
Pt_Pd_111_1	Pt_Pd_111_1	--	Ag_Cu_111_1L
Ir_Ag_111_1	Ir_Ag_111_1	Cu_Ag_100_1	Cu_Ag_100_1
Cu_Ir_111_1L	Cu_Ir_111_1L	Pd_Cu_100_1L	Pd_Cu_100_1L
Ir_Cu_111_1	Ir_Cu_111_1	Ag_Rh_100_1	Ag_Rh_100_1
Rh_Pd_100_1L	Rh_Pd_100_1L	Pt_Cu_100_1L	Pt_Cu_100_1L
Pd_100	Pd_100	Pt_Cu_111_1L	Pt_Cu_111_1L
Au_Pt_100_2	Au_Pt_100_2	Cu_Pd_100_1	Cu_Pd_100_1
Pt_Ag_100_4	Pt_Ag_100_4	Cu_Pd_100_2	Cu_Pd_100_2
Pt_Pd_100_4	Pt_Pd_100_4	Ag_Cu_100_2	Ag_Cu_100_2
Pd_Pt_100_1L	Pd_Pt_100_1L	--	Ag_Cu_100_1L
Ag_Pd_100_4	Ag_Pd_100_4	Cu_Ag_100_2	Cu_Ag_100_2
Pd_Au_100_2	Pd_Au_100_2	--	Rh_Cu_100_1L
Ag_Pt_111_3	Ag_Pt_111_3	Cu_Ag_100_4	Cu_Ag_100_4
Pt_Pd_100_1	Pt_Pd_100_1	Cu_Au_100_2	Cu_Au_100_2
Pt_Pd_111_1L	Pt_Pd_111_1L	Ag_Cu_111_3	Ag_Cu_111_3
Ag_Pt_100_2	Ag_Pt_100_2	Cu_Pd_100_4	Cu_Pd_100_4
Pt_Ag_100_1	Pt_Ag_100_1	--	Cu_Pt_100_2
Pd_Cu_111_2	Pd_Cu_111_2	--	Au_Ir_100_1
Pt_Rh_100_1	Pt_Rh_100_1	Au_Cu_111_3	--
Ag_Pt_111_2	Ag_Pt_111_2		
Pd_Ag_100_4	Pd_Ag_100_4		
Pd_Pt_100_1	Pd_Pt_100_1		
Pt_Pd_111_2	Pt_Pd_111_2		
Cu_Pt_100_1	Cu_Pt_100_1		
Pd_Ag_111_1	Pd_Ag_111_1		
Pt_111	Pt_111		
Pt_100	Pt_100		
Pd_Cu_100_2	Pd_Cu_100_2		
Pd_Pt_100_2	Pd_Pt_100_2		
Cu_Pt_100_4	Cu_Pt_100_4		
Ag_Pd_111_3	Ag_Pd_111_3		
Pt_Au_100_4	Pt_Au_100_4		

Pd_Pt_100_4	Pd_Pt_100_4	
Pd_Ag_100_1	Pd_Ag_100_1	
Pt_Ag_111_3	Pt_Ag_111_3	
Au_Pt_100_4	Au_Pt_100_4	
Au_Pd_111_3	Au_Pd_111_3	
Pd_Au_100_4	Pd_Au_100_4	
Pt_Pd_111_3	Pt_Pd_111_3	
Au_Pd_111_1L	Au_Pd_111_1L	
Ir_Au_111_1	Ir_Au_111_1	
Pt_Cu_100_1	Pt_Cu_100_1	
Pt_Au_111_3	Pt_Au_111_3	
Pd_Cu_100_4	Pd_Cu_100_4	
Au_Pd_100_4	Au_Pd_100_4	
Cu_Rh_111_1	Cu_Rh_111_1	
Pt_Cu_111_2	Pt_Cu_111_2	
Ag_Pd_100_1L	Ag_Pd_100_1L	
Pd_Cu_111_3	Pd_Cu_111_3	
Rh_Cu_100_1L	--	
Pd_Ag_111_3	Pd_Ag_111_3	
Pd_Cu_100_1	--	
Cu_Pt_100_2	--	
Au_Rh_100_1	Au_Rh_100_1	
Pt_Cu_100_2	Pt_Cu_100_2	
Au_Pt_111_3	Au_Pt_111_3	
Ir_Cu_100_1L	Ir_Cu_100_1L	
Pt_Pd_100_1L	Pt_Pd_100_1L	
Au_Pt_100_4	Au_Pt_100_4	
Rh_Au_111_1	Rh_Au_111_1	
Au_Pt_100_2	Au_Pt_100_2	
Ir_Pt_111_3	Ir_Pt_111_3	
Rh_Pt_100_1L	Rh_Pt_100_1L	
Pt_Pd_100_2	Pt_Pd_100_2	
Pt_Au_100_1	Pt_Au_100_1	
Pd_Ag_111_2	Pd_Ag_111_2	
Au_Pd_100_1L	Au_Pd_100_1L	
Pt_Ag_100_2	Pt_Ag_100_2	
Pd_Pt_111_1L	Pd_Pt_111_1L	
Ag_Rh_111_1	Ag_Rh_111_1	
Ag_Pd_111_1L	Ag_Pd_111_1L	
Pt_Cu_111_1	Pt_Cu_111_1	
Ir_Pt_111_1	Ir_Pt_111_1	
Cu_Pd_100_1L	Cu_Pd_100_1L	
--	Cu_Ir_111_1	
--	Pt_Ag_111_2	

--	Rh_Au_111_2	
--	Pt_Cu_111_3	
--	Ag_Ir_111_1	
--	Ir_Pd_100_1L	
--	Ir_Pt_100_1L	
--	Pd_Au_100_1	
--	Rh_Pd_111_1L	
--	Pt_Cu_100_4	
--	Pd_Pt_111_1	
--	Pd_Pt_111_2	
--	Pt_Au_111_2	
--	Pd_Cu_100_1	
--	Cu_Pt_100_1L	
--	Au_Rh_111_1	
--	Pd_Pt_111_3	
--	Au_Pt_100_1L	
--	Pt_Ag_111_1	
--	Pt_Rh_111_1	
--	Ir_Pd_111_1	

6. Validation analysis

7.

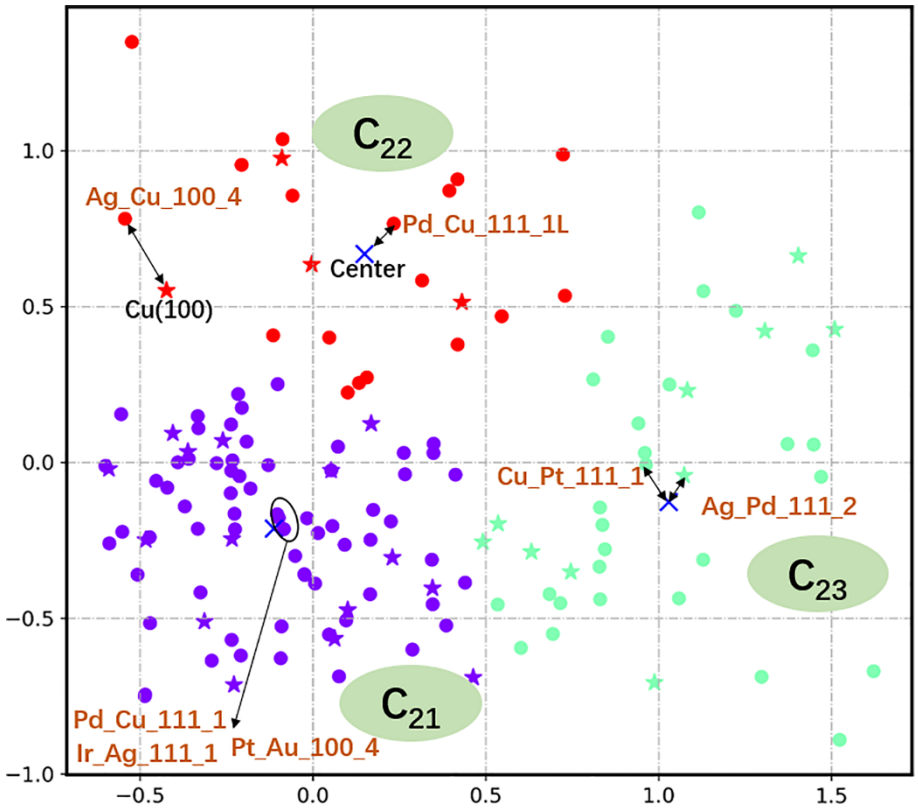

Fig. S6. The location of the ensembles as the validation samples of three clusters. Circle and pentagram points are for train and test data, respectively and X-type point are the centers of corresponding clusters.

Table S11. The distances (d_{center}) between every system and the center of the C_{21} cluster in the feature space.

Systems			d_{center}
-0.1131035	-0.211979029	Center	0
-0.0167341	-0.179353695	Pd_Ag_100_2	0.1017422
-0.1916611	0.066426622	Pt_Au_100_2	0.2892767
-0.5072928	-0.360498902	Pd_111	0.4212403
-0.2376922	-0.099057304	Au_Ir_111_1	0.1681477
0.34637804	-0.455521769	Au_Pt_111_2	0.520035
-0.1033132	-0.166690064	**Pd_Cu_111_1**	**0.0463351**
-0.1289592	-0.008840698	Ag_Pt_100_4	0.2037562
-0.5511725	-0.222856241	Ir_Pt_111_2	0.438204
-0.0930275	-0.628768775	Pt_Pd_111_1	0.417273
-0.0986524	-0.178175991	**Ir_Ag_111_1**	**0.0367625**
-0.4851277	-0.745184646	Cu_Ir_111_1L	0.6501617
-0.600187	-0.011421712	Ir_Cu_111_1	0.5267576
0.05638056	-0.204453527	Rh_Pd_100_1L	0.1696511
-0.3250793	-0.41739781	Pd_100	0.2951789
0.05297651	-0.02592314	Au_Pt_100_2	0.249398
-0.3329456	-0.213314456	Pt_Ag_100_4	0.2198461
-0.359124	0.01116127	Pt_Pd_100_4	0.3321411
-0.226771	-0.165115951	Pd_Pt_100_1L	0.1229489
0.26295136	0.030234115	Ag_Pd_100_4	0.447308
0.22554866	-0.189583585	Pd_Au_100_2	0.3393919
-0.2350033	-0.569594154	Ag_Pt_111_3	0.3778203
0.09627909	-0.507343185	Pt_Pd_100_1	0.3620512
0.00625462	-0.388903299	Pt_Pd_111_1L	0.2134211
0.26640587	-0.038311669	Ag_Pt_100_2	0.417358
0.28776049	-0.600790548	Pt_Ag_100_1	0.55845
-0.2785745	-0.00280235	Pd_Cu_111_2	0.2667124
-0.4721816	-0.240112989	Pt_Rh_100_1	0.3601785
0.34391239	-0.312540432	Ag_Pt_111_2	0.4679489
-0.2253318	-0.214773742	Pd_Ag_100_4	0.1122631
-0.0907389	-0.526371925	Pd_Pt_100_1	0.3151874
-0.2085094	-0.619932409	Pt_Pd_111_2	0.4189609
0.07255406	0.050219604	Cu_Pt_100_1	0.3212738
0.04650203	-0.552603292	Pd_Ag_111_1	0.3761633
0.07549619	-0.686915964	Pt_111	0.5110136
-0.2056384	0.174952026	Pt_100	0.3978421
-0.2123387	-0.044220206	Pd_Cu_100_2	0.1949119
-0.4534166	-0.059403891	Pd_Pt_100_2	0.3729506
-0.2359492	-0.027267972	Cu_Pt_100_4	0.2218315
0.01493719	-0.226967159	Ag_Pd_111_3	0.128915
-0.0838911	-0.214338217	**Pt_Au_100_4**	**0.0293075**

-0.4211357	-0.081293006	Pd_Pt_100_4	0.3346082
0.38565317	-0.523486052	Pd_Ag_100_1	0.5880433
-0.470955	-0.516070986	Pt_Ag_111_3	0.4696058
-0.331136	0.1093348	Au_Pt_100_4	0.388305
-0.0512143	-0.300342848	Au_Pd_111_3	0.1078816
0.09198448	-0.264539564	Pd_Au_100_4	0.2117161
-0.292701	-0.636357672	Pt_Pd_111_3	0.4608172
-0.3705051	-0.141494698	Au_Pd_111_1L	0.2668775
0.16661799	-0.248453655	Ir_Au_111_1	0.2820896
-0.0234308	-0.361832332	Pt_Cu_100_1	0.1746345
0.44016747	-0.386062612	Pt_Au_111_3	0.580012
-0.3907132	-4.87E-05	Pd_Cu_100_4	0.3492587
0.41230923	-0.039631287	Au_Pd_100_4	0.5529578
-0.3330483	0.148185325	Cu_Rh_111_1	0.4220119
-0.5888055	-0.260085662	Pt_Cu_111_2	0.4781283
-0.1805339	-0.084157653	Ag_Pd_100_1L	0.144517
-0.236714	0.121495759	Pd_Cu_111_3	0.3556473
-0.1018485	0.250715342	Rh_Cu_100_1L	0.4628312
-0.0247813	-0.359128775	Pd_Ag_111_3	0.1716213
0.16554805	-0.423188437	Pd_Cu_100_1	0.3496514
-0.2162045	0.218793441	Cu_Pt_100_2	0.4429388
0.34861925	0.029901557	Au_Rh_100_1	0.5212429
-0.554619	0.154326659	Pt_Cu_100_2	0.5736861
-0.4860763	-0.750065724	Au_Pt_111_3	0.6547106
0.34913008	0.059627928	Ir_Cu_100_1L	0.5361252
0.17425198	-0.152559403	Pt_Pd_100_1L	0.2934346
-0.2328198	0.006181269	Au_Pt_100_4	0.2488491
-0.260226	0.069544572	Rh_Au_111_1	0.3176485
0.05297651	-0.02592314	Au_Pt_100_2	0.249398
-0.5898357	-0.020666519	Ir_Pt_111_3	0.5136867
0.10081681	-0.473995856	Rh_Pt_100_1L	0.3382525
-0.4049053	0.093467622	Pt_Pd_100_2	0.4224286
0.46362658	-0.690399959	Pt_Au_100_1	0.7493358
0.06292584	-0.565620686	Pd_Ag_111_2	0.3950301
0.2299573	-0.305767948	Au_Pd_100_1L	0.3556502
-0.3613919	0.034358948	Pt_Ag_100_2	0.3497564
-0.2282419	-0.713641733	Pd_Pt_111_1L	0.5147061
0.16867346	0.124065877	Ag_Rh_111_1	0.4385481
-0.2340107	-0.245666748	Ag_Pd_111_1L	0.1255125
-0.3137514	-0.510716723	Pt_Cu_111_1	0.3598663
-0.4834146	-0.248911509	Ir_Pt_111_1	0.3721482
0.34590526	-0.403770957	Cu_Pd_100_1L	0.4974668

Table S12. The reaction barriers and reaction enthalpy (E_a and E_{enth}) of key elementary

steps (ES) and desorption energy (E_{de}) of products for NH_3-SCO on Cu(100), Pt_Au_100_4 and Pd_Cu_111_1 (Units of E_a, E_{enth} and E_{de}: eV).

	Pt_Au_100_4			Pd_Cu_111_1		
ES	E_a	E_{enth}	E_{de}	E_a	E_{enth}	E_{de}
$NH_3^*+O^*=NH_2^*+OH^*$	1.15	0.05	--	1.17	0.51	--
$N^*+N^*=N_2+2*$	1.39	-1.83	0.41	1.89	-1.14	0.33
$N^*+O^*=NO^*+*$	1.80	-0.72	0.42	2.06	-0.13	2.18
$N^*+NO^*=N_2O^*+*$	2.07	0.59	0.04	2.11	0.99	0.14

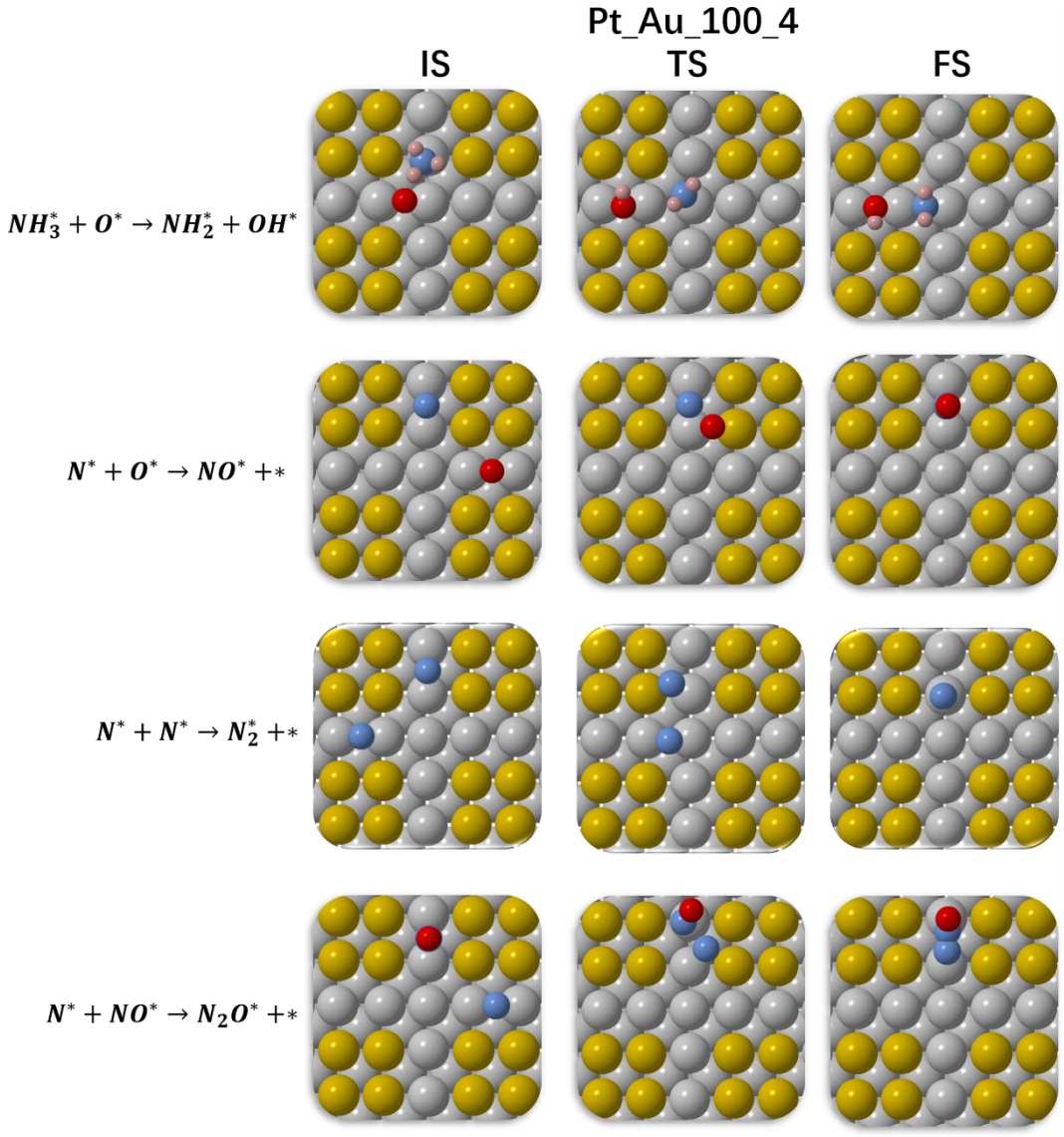

Fig. S7. The configurations of initial, transition and final states (IS, TS and FS) of primary elementary steps of simplified NH_3-SCO process on Pt_Au_100_4 system.

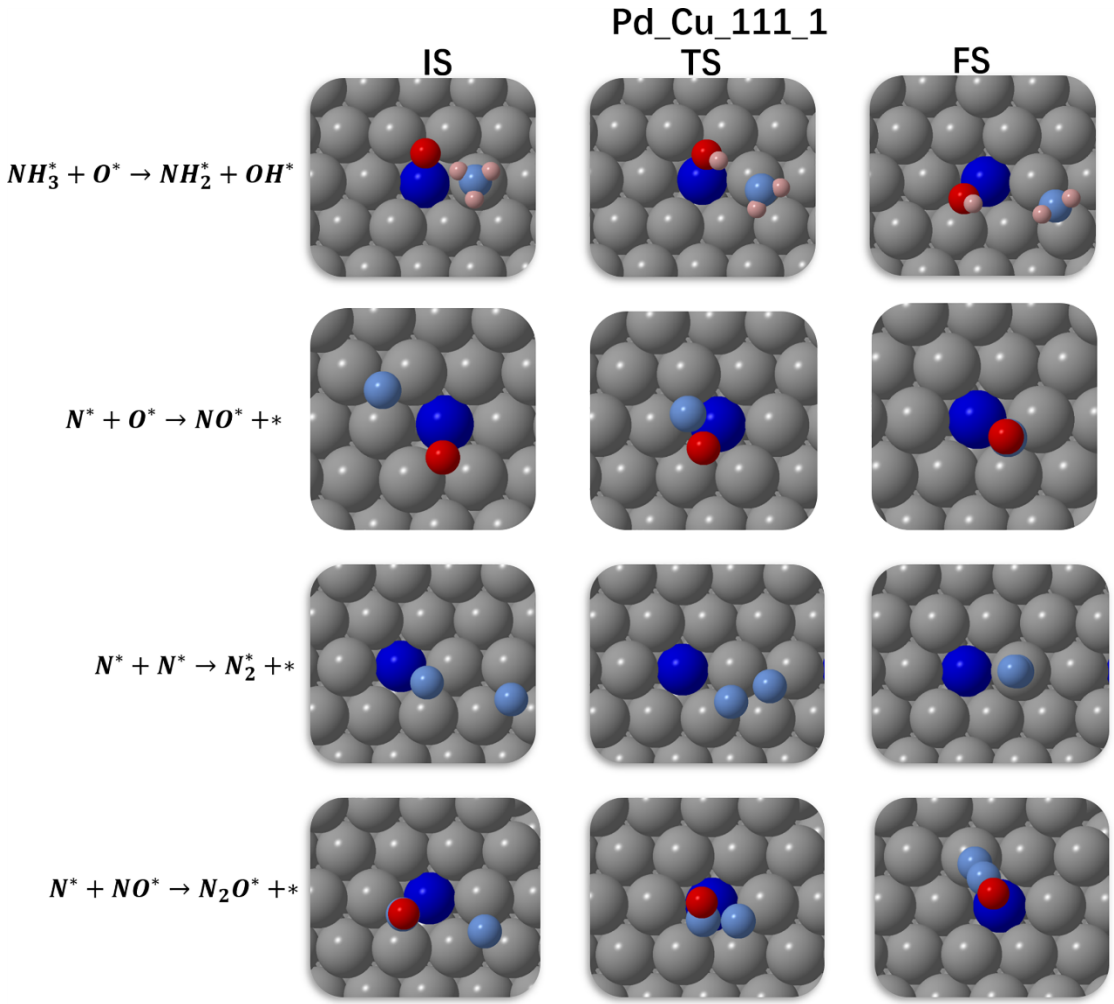

Fig. S8. The configurations of initial, transition and final states (IS, TS and FS) of primary elementary steps of simplified NH_3-SCO process on Pd_Cu_111_1 system.

Table S13. The distances (d_{center}, $d_{Cu(100)}$) between every system and the center of the C_{22} cluster or Cu(100) in the feature space.

Systems			d_{center}	$d_{Cu(100)}$
0.149029235	0.668409	Center	0	0.584277
0.723212697	0.98735	Au_Cu_111_3	0.656818	1.226723
0.546148702	0.468645	Cu_Ag_100_4	0.444533	0.973049
0.31579723	0.583225	Cu_Ag_100_2	0.187264	0.739873
-0.058948732	0.855538	Rh_Cu_111_1L	0.279772	0.474753
-0.523506637	1.348645	Au_Cu_111_1L	0.95657	0.80363
0.418729288	0.377759	Cu_Ag_100_1	0.396504	0.859806
0.39468872	0.871304	Ag_Cu_111_3	0.318614	0.878444
-0.087656813	1.036574	Pt_Cu_111_1L	0.437682	0.590109
-0.206182506	0.954401	Cu_Ag_111_1L	0.456034	0.457916
-0.115019891	0.407205	Cu_Pd_100_2	0.371415	0.340361
0.41818994	0.908041	Ag_Cu_100_2	0.360376	0.914074
0.100793623	0.223938	Cu_Pd_100_1	0.447081	0.617992
0.729039974	0.534381	Cu_Au_100_2	0.595295	1.15255
0.13333044	0.25469	Cu_Pd_100_4	0.414017	0.63079
0.156116924	0.272205	Ag_Rh_100_1	0.396267	0.643198
0.047356276	0.400224	Pd_Cu_100_1L	0.286811	0.494383
-0.543410033	0.781383	**Ag_Cu_100_4**	0.701595	**0.259529**
0.233847033	0.765854	**Pd_Cu_111_1L**	**0.129188**	0.691375
-0.089892032	0.975566	Ir_Cu_111_1L	0.389138	0.539667
-0.423385923	0.551276	Cu_100	0.584277	0
-0.003407145	0.634811	Au_Cu_100_1L	0.156095	0.428206
0.430904777	0.513669	Pt_Cu_100_1L	0.321556	0.855118

Table S14. The reaction barriers and reaction enthalpy (E_a and E_{enth}) of key elementary steps (ES) and desorption energy (E_{de}) of products for NH_3-SCO on Cu(100), Pd_Cu_111_1L and Ag_Cu_100_4 (Units of E_a, E_{enth} and E_{de}: eV).

	Cu(100)			**Pd_Cu_111_1L**			**Ag_Cu_100_4**		
ES	E_a	E_{enth}	E_{de}	E_a	E_{enth}	E_{de}	E_a	E_{enth}	E_{de}
$NH_3^*+O^*=NH_2^*+OH^*$	0.92	-0.03	--	0.85	-0.14	--	0.29	-0.58	--
$N^*+N^*=N_2+2*$	2.39	-1.08	--	1.46	-2.49	0.22	1.49	-2.22	0.19
$N^*+O^*=NO^*+*$	2.69	1.30	1.21	2.07	0.31	1.339	2.00	0.81	1.31
$N^*+NO^*=N_2O^*+*$	1.15	0.00	--	0.95	-0.68	0.138	0.68	-1.05	0.704

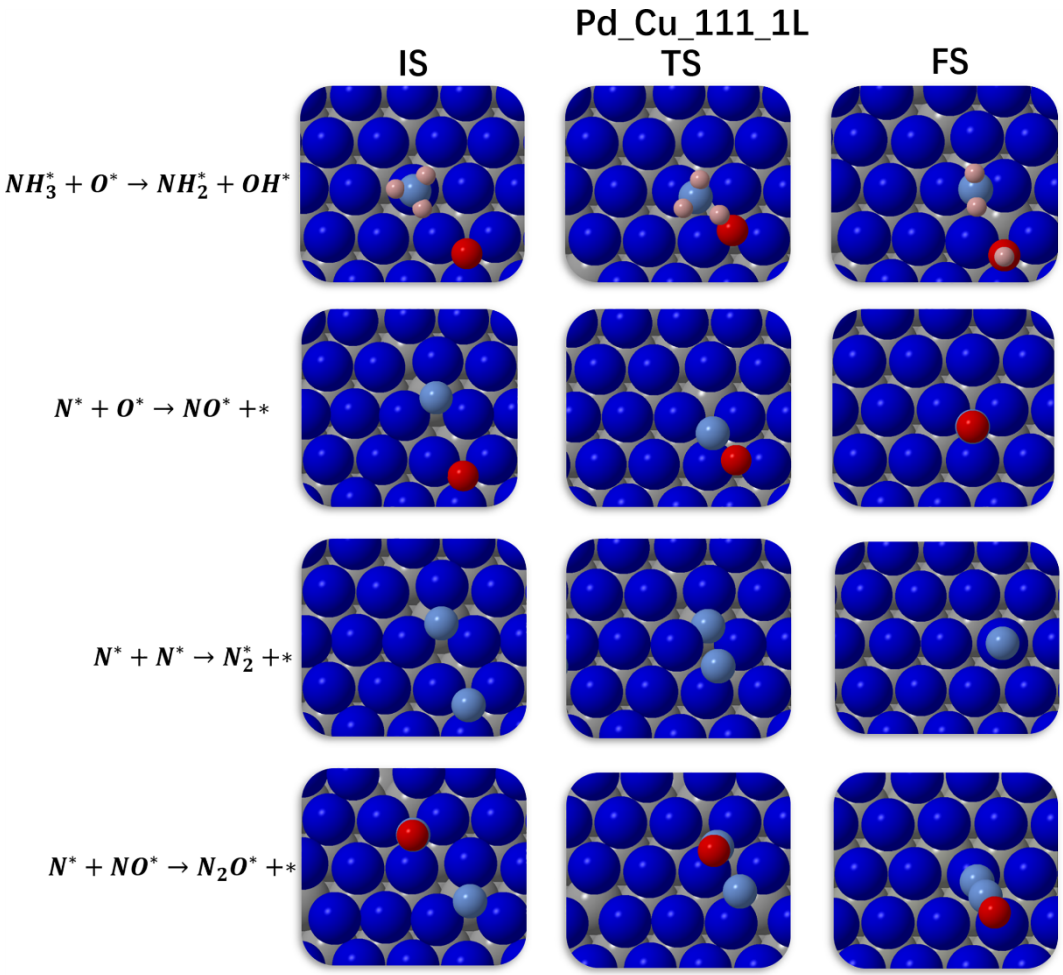

Fig. S9. The configurations of initial, transition and final states (IS, TS and FS) of primary elementary steps of simplified NH_3-SCO process on Pd_Cu_111_1L system.

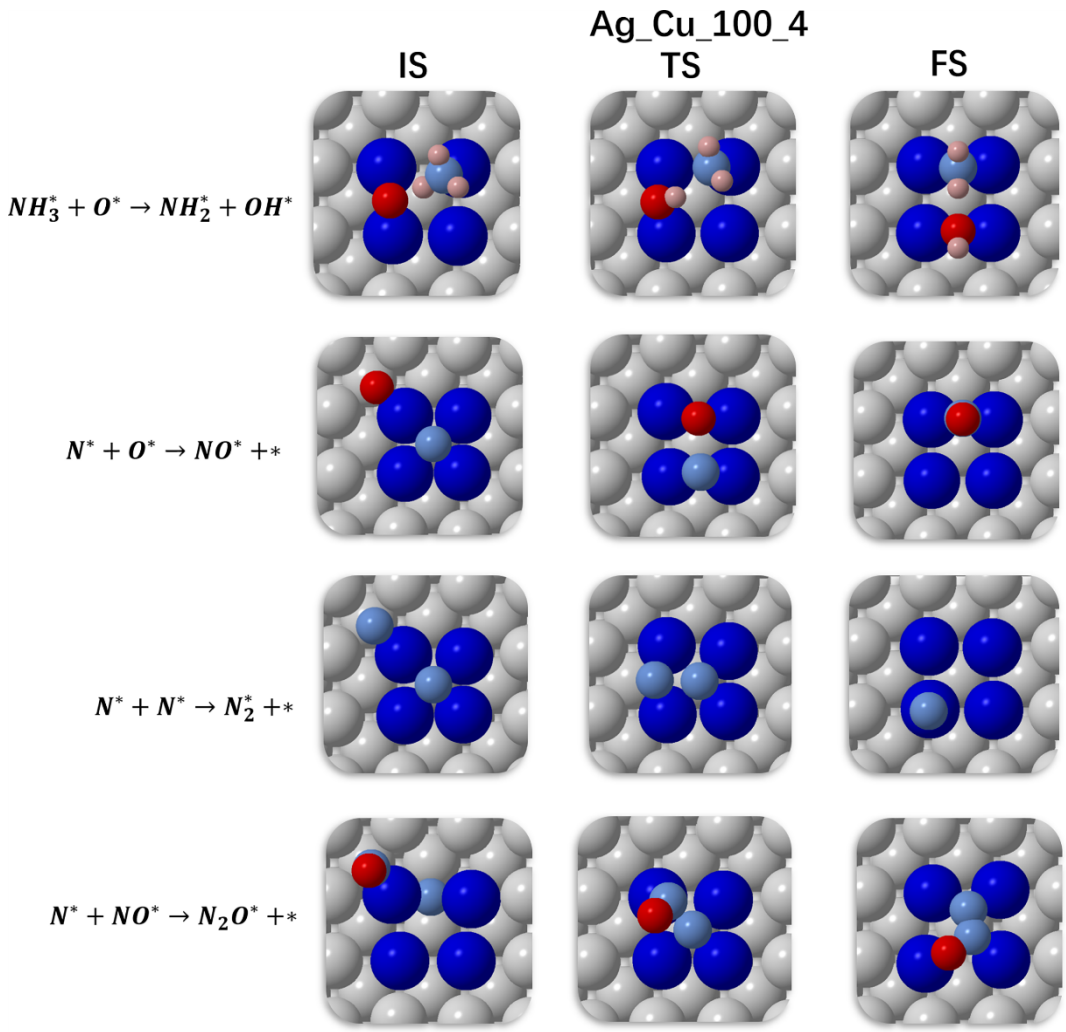

Fig. S10. The configurations of initial, transition and final states (IS, TS and FS) of primary elementary steps of simplified NH_3-SCO process on Ag_Cu_100_4 system.

Table S15. The distances (d_{center}) between every system and the center of the C_{23} cluster in the feature space.

	Systems		d_{center}
1.02849922	-0.126545316	Center	0
0.94154816	0.124899339	Cu_Pd_111_2	0.2660543
0.83030616	-0.144882048	Pd_Au_111_3	0.1990395
1.62174265	-0.670195267	Ir_Pt_111_1L	0.8046695
1.52370707	-0.890336474	Cu_Pt_111_1L	0.9102789
1.12925843	0.549110863	Cu_111	0.6831279
1.44837815	0.05688678	Ag_Pt_100_1	0.4581983
0.96007319	0.03014914	Cu_Pd_111_3	0.1709833
1.05880081	-0.436592212	Cu_Pt_111_3	0.3115241
1.22369423	0.485949936	Cu_Ag_111_1	0.6428464
1.44565148	0.359323905	Cu_Ag_111_3	0.6403787
0.68434986	-0.422857487	Pt_Au_111_2	0.4541362
1.29760496	-0.688321774	Rh_Pt_111_1L	0.622905
0.5344846	-0.456336859	Cu_Pt_100_1L	0.5939806
0.69394883	-0.550721583	Ir_Pt_100_1L	0.5402309
1.03123329	0.249542159	Ag_Pd_100_2	0.3760974
0.84456955	-0.27898223	Ir_Pd_111_1L	0.2388873
0.82886363	-0.335015411	Pd_Au_111_2	0.2886419
0.71554252	-0.451780227	Pt_Ag_111_1	0.4513531
0.81059864	0.265892865	Cu_Au_100_1	0.4488746
0.83075789	-0.439400727	Pd_Au_111_1	0.3701083
1.11585772	0.801838502	Ag_Cu_111_2	0.9324849
1.37262665	0.058838173	Au_Pd_100_2	0.3908845
0.85337227	0.402660325	Cu_Au_100_4	0.5574299
0.83739107	-0.200816316	Cu_Pt_111_2	0.2050329
0.96340752	-0.007584168	**Cu_Pt_111_1**	**0.1356049**
0.60160412	-0.5954729	Pd_Au_100_1	0.6341392
1.12871814	-0.312630735	Au_Pd_111_2	0.2113566
1.46988646	-0.046434415	Au_Pt_100_1	0.4485983
1.40387493	0.662450745	Ag_Cu_100_1	0.8737401
1.30723669	0.4208852	Cu_Ag_111_2	0.6143084
1.50949341	0.426317678	Cu_Au_111_1	0.7328116
0.98787053	-0.706739677	Pt_Au_111_1	0.5816152
0.53560459	-0.196892451	Au_Rh_111_1	0.4978894
1.07390175	-0.042015535	**Ag_Pd_111_2**	**0.0959514**
0.74593216	-0.351505911	Rh_Pd_111_1L	0.3611806
1.082883	0.230546993	Cu_Pd_111_1	0.3612098
0.4915884	-0.255544492	Pt_Ag_111_2	0.5521902
0.6320079	-0.287284207	Ir_Pd_100_1L	0.4278345

Table S16. The reaction barriers and reaction enthalpy (E_a and E_{enth}) of key elementary steps (ES) and desorption energy (E_{de}) of products for NH_3-SCO on Cu_Pt_111_1 (Units of E_a, E_{enth} and E_{de}: eV).

	Cu_Pt_111_1		
ES	E_a	E_{enth}	E_{de}
$NH_3^*+O^*=NH_2^*+OH^*$	0.61	0.22	--
$N^*+N^*=N_2+2*$	1.57	-3.17	0.13
$N^*+O^*=NO^*+*$	1.47	-0.32	1.28
$N^*+NO^*=N_2O^*+*$	0.5	-0.65	-0.62

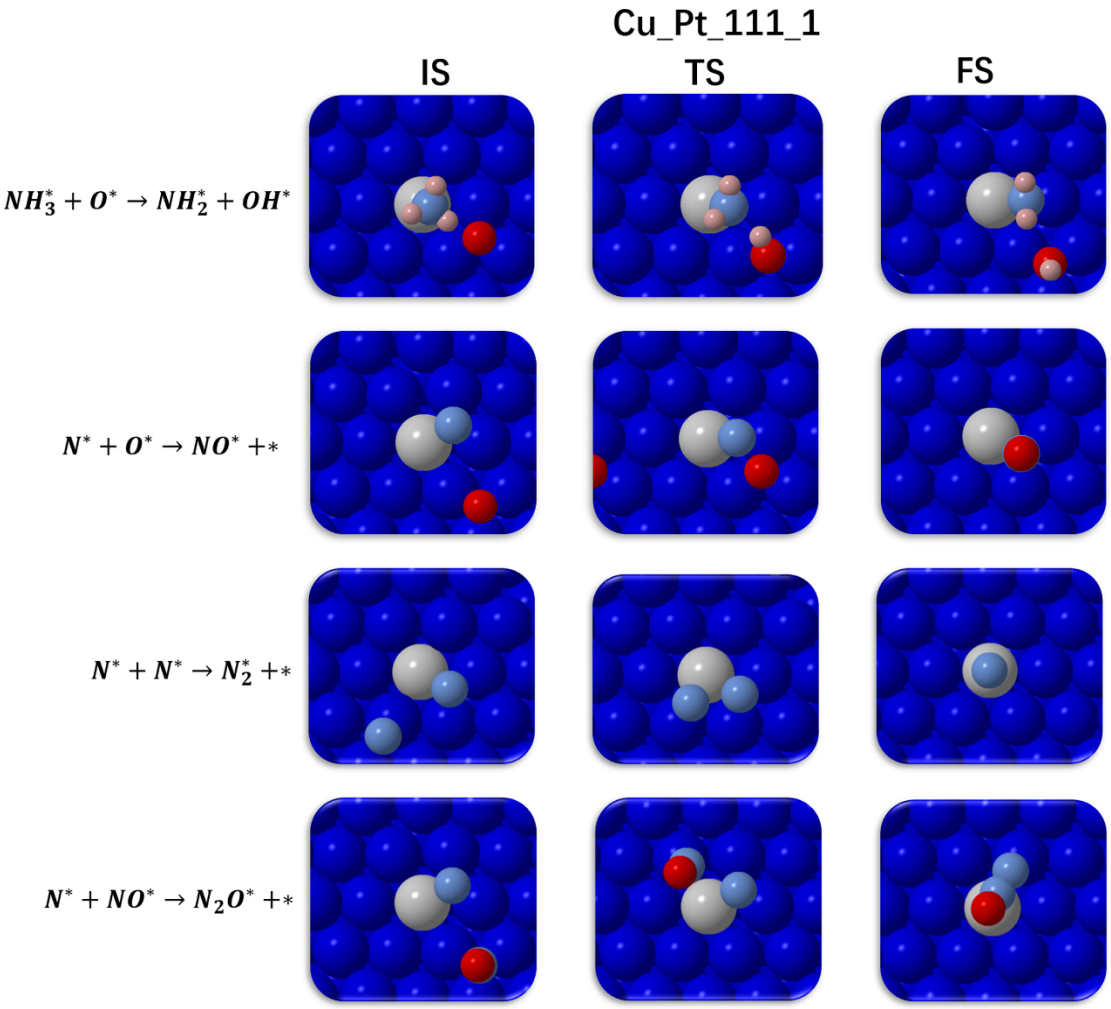

Fig. S11. The configurations of initial, transition and final states (IS, TS and FS) of primary elementary steps of simplified NH_3-SCO process on Cu_Pt_111_1 system.

References:

1. H. Ma, W. F. Schneider, *ACS Catal.,* 2019, **9**, 2407−2414.
2. Z. Jiang, P. Qin, T. Fang, *Chem. Phys.,* 2014, **445**, 59–67.
3. J. Pérez-Ramírez, E. V. Kondratenko, G. Novell-Leruth, J. M. Ricart, *J. Catal.,* 2009, **261**, 217–223.
4. N. López, M. García-Mota, J. Gómez-Díaz, *J. Phys. Chem. C*, 2008, **1**, 112.
5. D. Yuan, X. Gong, and R. Wu, *Phys. Rev. B*, 2007, **75**, 085428.
6. H. Zhuang, A. J. Tkalych, E. A. Carter, *J. Phys. Chem. C*, 2016, **120**, 23698.23706.
7. R. Tran, Z. Xu, B. Radhakrishnan, D. Winston, W. Sun, K. A. Persson, S. P. Ong, *Sci. Data*, 2016, **3**, 160080.

Appendix:

Considering a lot of adsorption configurations may change for each system after optimization and would cause many same or similar binding configurations for every species, we have developed a python-based procedure to fast check slab models and extract the information of surface and adsorbates. The procedure mainly consists of the two base functions: *distinguish_atom_binding* and *get_binding_adatom*. The *distinguish_atom_binding* could effectively distinguish the types of atoms: adsorbates, surface atoms and subsurface atoms and output the corresponding atomic symbols and the serial number of every atom in the configurations. Based that, the *get_binding_adatom* mainly extract the information of binding sites and atoms: the atom of the adsorbate binding to surface atoms, binding type of the adsorbate and surface atoms binding to the adsorbate. Taking a binding configuration of NH_2 on Pd_Cu_111_1 ensemble (in Fig. A1) as the typical example, related attribution and information could be obtained, as shown in Table A1.

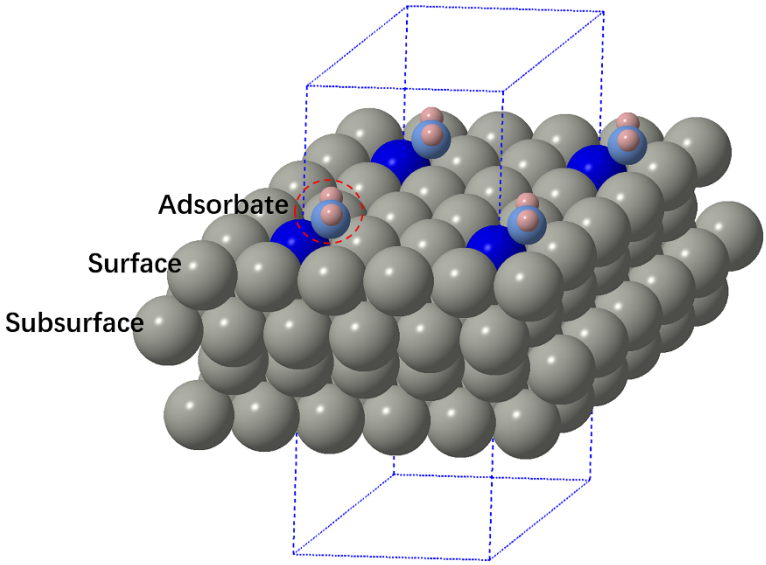

Fig. A1. The typical configuration of NH_2 on Pd_Cu_111_1 ensemble.

Table A1. Related information extracted from the configuration of NH_2 on Pd_Cu_111_1 ensemble.

Attribution	Information
Surface atoms	Pd, Pd, Pd, Pd, Pd, Pd, Pd, Pd, Cu
Subsurface atoms	Pd, Pd, Pd, Pd, Pd, Pd, Pd, Pd, Pd
Adsorbate	NH_2
The atom of the adsorbate binding to surface atoms	N
Binding type of the adsorbate	bridge
Surface atoms binding to the adsorbate	Pd, Cu

Base function 1:

```
from catkit.gen.utils import get_unique_coordinates
import numpy as np
def distinguish_atom_binding(poscar,tol_layer=0.01,tol=0.05,base_layer=4,atoms_layer=9):
    '''
    To distinguish the atoms at different layer
    Parameters:
    ----------------------
    poscar:
       atoms objects
    tol:
       tolerance whether atoms in the same layer
    layer:
       layer number; eg. surface atoms:'surf_atom',subsurface atom:'subsurf_atom',
       adsorb layer:'adatom,others could be represented by the corresponding number
    base_layer:
       the layer of the substrate
    ----------------------
    '''
    if isinstance(poscar, str):
       struct=read(poscar,format='vasp')
    else:
       struct=poscar
    #the representative Z coords of every layer
    coordinates_layer=get_unique_coordinates(struct,axis=2, tag=True, tol=tol_layer)
    coordinates=struct.get_scaled_positions()[:,2]
    #the dict about the atoms and corresponding layers
    key_atom=[]
    value_layer=[]
    #print(coordinates_layer)
    for i,coord in enumerate(coordinates):
        for j,coord_layer in enumerate(coordinates_layer):
            dis=np.abs(coord-coord_layer)
            if dis < tol:
               #print(f'atom {i+1} belongs to layer {j+1}')
               key_atom += [i]
               value_layer += [j+1]
               break
            elif j >= base_layer:
```

```
                #print(f'atom {i+1} belongs to layer {j+1}')
                key_atom += [i]
                value_layer += [j+1]

    #if len(key_atom) != (i+1):
    #   raise ValueError('tol is too large and not to distinguish the layers; Please reduce tol!')
    dict_atom_layer=dict(zip(key_atom,value_layer))
    #print(dict_atom_layer)
    adatoms,adatoms_symb=[],[]
    surfatoms,surfatoms_symb=[],[]
    subsurfatoms,subsurfatoms_symb=[],[]
    for k in range(len(coordinates)):
        #print(dict_atom_layer.get(k))
        if int(dict_atom_layer.get(k)) > base_layer:
            dict_atom_layer[k] = 'adatom'
            adatoms += [k]
            adatoms_symb += [struct.get_chemical_symbols()[k]]
        elif dict_atom_layer.get(k) == base_layer:
            dict_atom_layer[k] = 'surf_atom'
            surfatoms += [k]
            surfatoms_symb += [struct.get_chemical_symbols()[k]]
        elif dict_atom_layer.get(k) == (base_layer-1):
            dict_atom_layer[k] = 'subsurf_atom'
            subsurfatoms += [k]
            subsurfatoms_symb += [struct.get_chemical_symbols()[k]]
        else:
            continue
    #print(dict_atom_layer)
    base_element=['Au','Ag','Pd','Pt','Rh','Ru','Ir','Cu','Fe','Co','Ni','Zn','Ti','Y','Zr','Nb','Mo','Tc','Hf','Ta','W','Re','Sc','V','Cr','Mn']
    if len(surfatoms) > int(atoms_layer):
       #print('surface atoms >9')
       #print(surfatoms_symb)
       surfatoms_final,surfatoms_symb_final=[],[]
       tmp=[]
       for n,atom_symb in enumerate(surfatoms_symb):
           if atom_symb not in base_element:
              #print(atom_symb)
              adatoms += [surfatoms[n]]
              adatoms_symb += [atom_symb]
              #surfatoms.pop(n)
              #surfatoms_symb.pop(n)
```

```
            tmp+=[n]
        for m,atom_symb in enumerate(surfatoms_symb):
            if m not in tmp:
                surfatoms_final += [surfatoms[m]]
                surfatoms_symb_final += [surfatoms_symb[m]]
        surfatoms=surfatoms_final
        surfatoms_symb=surfatoms_symb_final
        #print(surfatoms_symb)
        ### Ignore structures where Z coord of adatoms < Z coord of surfatoms
        Z_mean=np.mean([struct.get_scaled_positions()[i][2] for i in surfatoms])
        Z_adatom=np.mean([struct.get_scaled_positions()[i][2] for i in adatoms])
        if Z_adatom <= Z_mean:
            surfatoms=[]
            surfatoms_symb=[]
    ### Ignore the structures without standard and integrated surface configurations
    elif len(surfatoms) < int(atoms_layer):
        #raise ValueError(f'{poscar} can not been analyzed!')
        surfatoms=[]
        surfatoms_symb=[]
    return adatoms,adatoms_symb,surfatoms,surfatoms_symb,subsurfatoms,subsurfatoms_symb
```

Base function 2:

```
def get_binding_adatom(poscar):
    # extract surface atoms and adsorbed atoms
    #adatoms,adatoms_symb=distinguish_atom_binding(poscar,tol=0.05,layer='adatom')
    #surf_atoms,surf_atom_symb=distinguish_atom_binding(poscar,tol=0.05,layer='surf_atom')

    # neighbor list of atoms in struct
    if isinstance(poscar, str):
        struct=read(poscar,format='vasp')
    else:
        struct=poscar
    adatoms,adatoms_symb,surfatoms,surfatoms_symb,subsurfatoms,subsurfatoms_symb=distinguish_atom_binding(poscar,tol=0.05)
    #print(adatoms_symb,surfatoms_symb)
    #print(struct.symbols)
    cutOff = natural_cutoffs(struct,mult=1.0)
```

```
    #print(cutOff)
    nl = NeighborList(cutOff, self_interaction=False, bothways=True)
    nl.update(struct)
    #### extract the adatoms binded with surface and corresponding surface atoms
    bind_adatoms=[]
    bind_adatoms_symb=[]
    bind_surfatoms=[]
    bind_surfatoms_symb=[]
    site_type=[]
    site_type2=[]
    site_type_symb=[]
    ### Extract the binded surface atoms and binded adsorbed atoms
    for i,atom in enumerate(adatoms):
        indices, offsets = nl.get_neighbors(atom)
        tmp=[]
        tmp2=[]
        #print(indices)
        for index in indices:
            #print(index)
            if index in surfatoms:
               bind_adatoms += [atom]
               tmp += [index]
               tmp2 += [struct.get_chemical_symbols()[index]]
            else:
               continue
        #tmp3_symb=[struct.get_chemical_symbols()[i] for i in tmp3]
        if tmp != []:
           bind_surfatoms += [tmp]
           bind_surfatoms_symb += [tmp2]
           site_type += [len(tmp2)]
        #print(struct.get_scaled_positions()[atom][0:-1])
    bind_adatoms=list(set(bind_adatoms))
    bind_adatoms_symb=[struct.get_chemical_symbols()[i] for i in bind_adatoms]
    ### Extract the bind type
    item=[]
    bind_type_symb = []
    for j,adatom in enumerate(bind_adatoms):
         p1=struct.get_scaled_positions()[adatom][0:-1]
         item_tmp=[]
```

```
        for k,atom in enumerate(subsurfatoms):
            p2=struct.get_scaled_positions()[atom][0:-1]
            if abs(p1[0]-p2[0])<0.025 and abs(p1[1]-p2[1])<0.025:
               item_tmp +=[True]
            else:
               item_tmp +=[False]
        if any(item_tmp):
           item +=[int(1)]
        else:
           item +=[int(0)]
    #print(item)
    typ={0:None,1:'top',2:'bri',3:'hol',4:'4-fold'}
    for m,bind in enumerate(site_type):
        bind_type=typ.get(bind)
        if bind_type == 'hol' and item[m]==0:
           bind_type_symb += ['fcc']
        elif  bind_type == 'hol' and item[m]==1:
           bind_type_symb += ['hcp']
        else:
           bind_type_symb += [bind_type]

    ### Extract the adsorbed species
    adspecie=[]
    for i,atom in enumerate(bind_adatoms):
        indices, offsets = nl.get_neighbors(atom)
        tmp3=[atom]
        #print(indices)
        for index in indices:
            if (index in surfatoms) or (index in subsurfatoms):
               continue
            else:
               tmp3+=[index]
        #print(tmp3)
        tmp3_symb=''.join(list([struct.get_chemical_symbols()[i]
   for i in tmp3]))
        Ele=list(dict(Counter(tmp3_symb)).keys())
        Num=list(dict(Counter(tmp3_symb)).values())
        #print(tmp3_symb)
        #print(Ele)
        mol='*'
        for j,E in enumerate(Ele):
            mol=mol+E
            if Num[j] == 1:
               continue
```

```
            else:
                mol=mol+str(Num[j])
        if mol == '*OH2':
            mol='*H2O'
        else:
            adspecie +=[mol.split('*')[1]]
        #adspecie+=[''.join(list(chain.from_iterable(zip(Ele,Num))
    ))]
        #mol=molecule(tmp3_symb)[0]
        #print(mol.symbol)
    return bind_adatoms,bind_adatoms_symb,adspecie,bind_type_sym
    b,bind_surfatoms,bind_surfatoms_symb
```