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Supporting Information

NO Dissociation on Platinum and Platinum-Rhodium Alloy: A Theoretical Investigation

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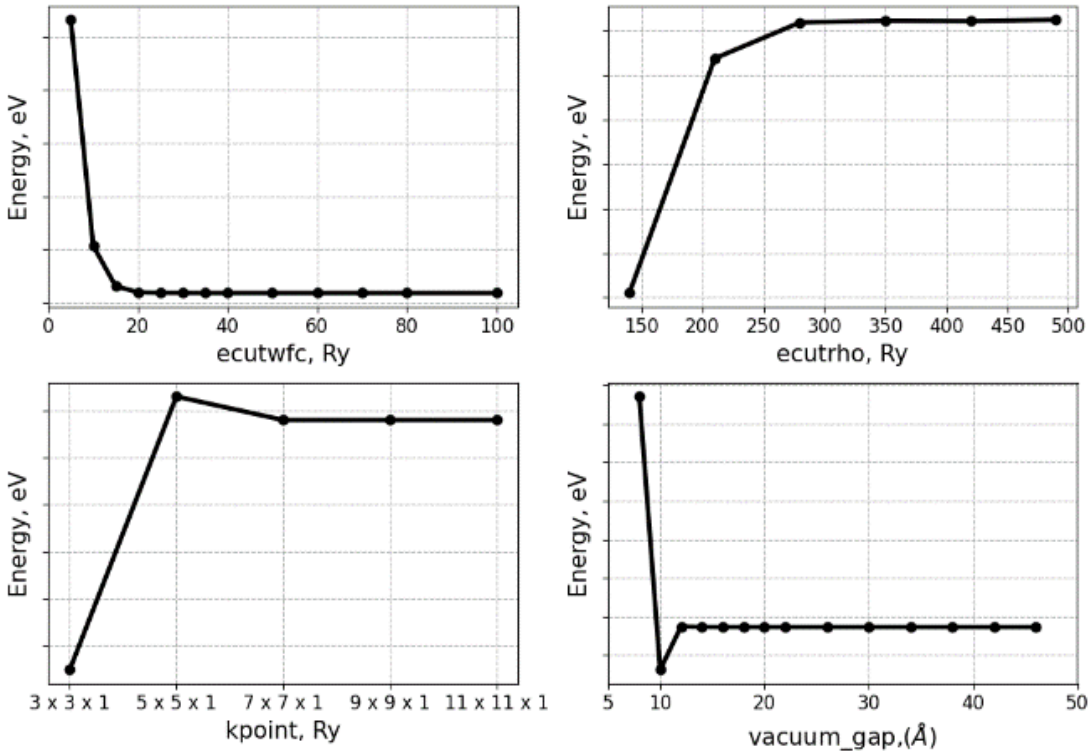

Figure 1S. The convergence tests for Pt (111) slab.

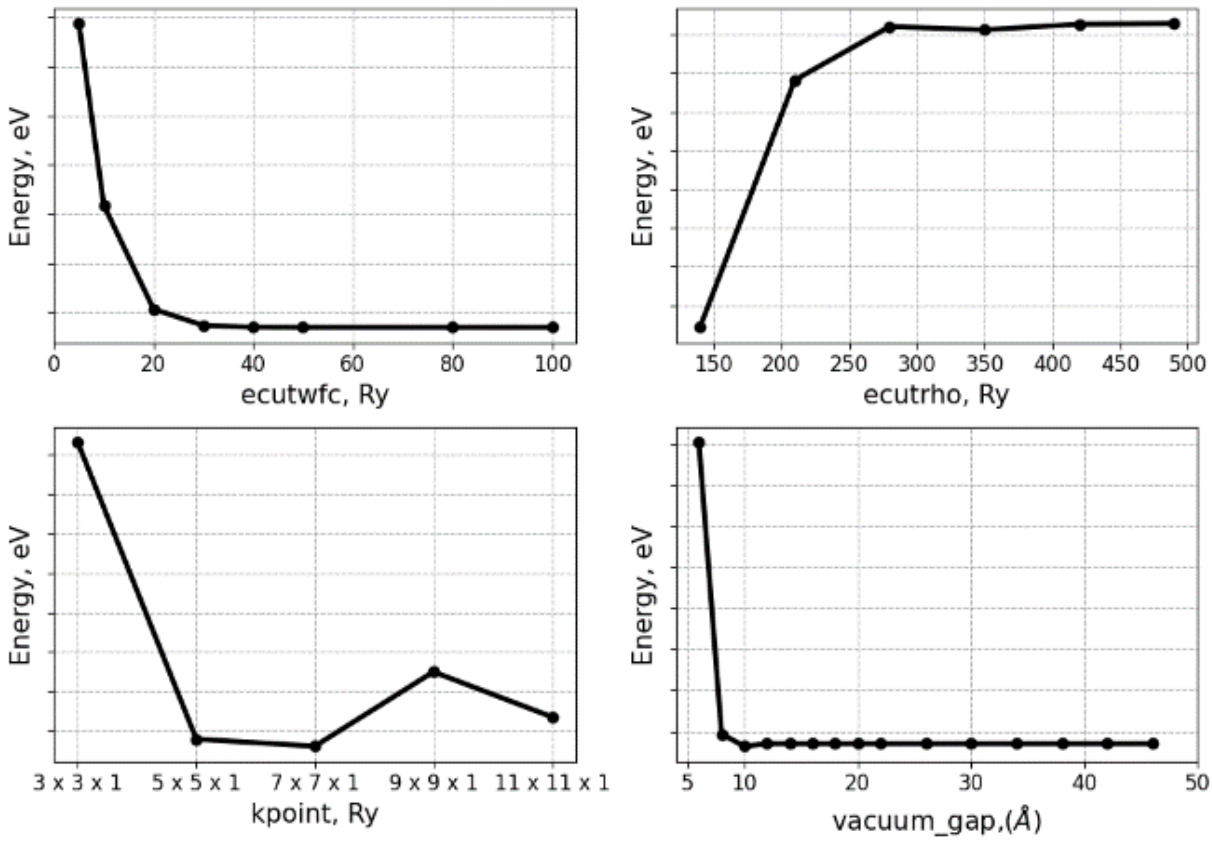

Figure 2S. The convergence tests for Rh_3Pt (111) slab.

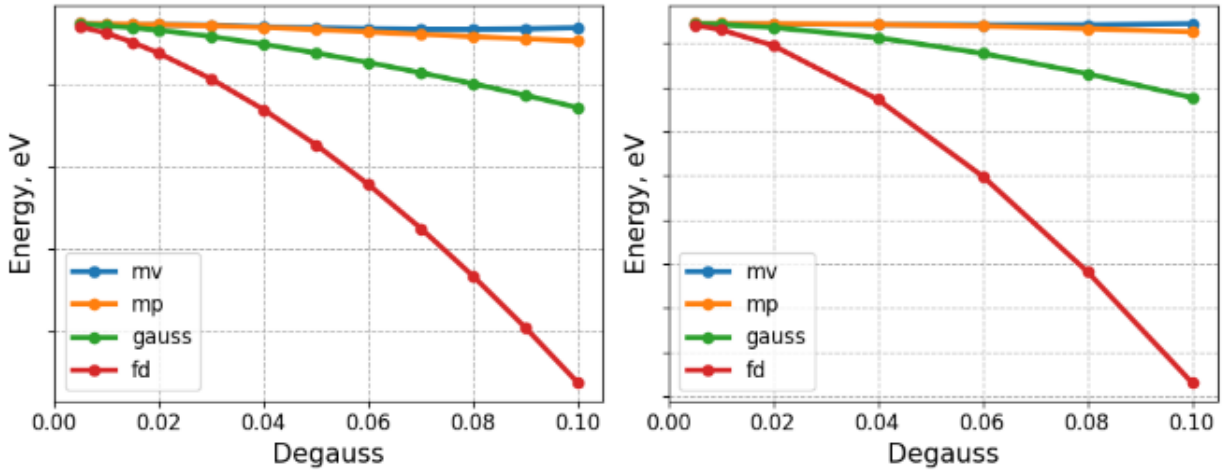

Figure 3S. Convergence test for smearing type for Pt (111) (left) and Rh_3Pt (111) (right).

Table S1. Phonon vibrations of transition state, initial state, and final state of reaction: NO* ---> N* + O* on the Pt (111) surface

Phonon calculation, Transition state			Phonon calculation Initial state		Phonon calculation Final state		Phonon calculation, Pt(111) slab	
mode	[cm^{-1}]	[THz]	[cm^{-1}]	[THz]	[cm^{-1}]	[THz]	[cm^{-1}]	[THz]
1	-450.44	-13.5038	0	0	0	0	-0.00	0.0000
2	-0.00	-0.0000	0	0	0	0	-0.00	0.0000
3	-0.00	-0.0000	0	0	0	0	0.00	0.0000
4	0.00	0.0000	37.61	1.1275	30.9	0.9265	74.51	2.2337
5	28.22	0.8460	58.15	1.7433	37.9	1.1361	77.38	2.3198
6	32.76	0.9822	69.07	2.0708	46.2	1.385	80.35	2.4087
7	46.52	1.3948	73.09	2.1913	49.75	1.4914	93.04	2.7892
8	49.64	1.4880	77.51	2.3236	60.85	1.8242	102.94	3.0862
9	56.09	1.6815	80.58	2.4156	63.98	1.918	104.51	3.1331
10	58.18	1.7443	83.34	2.4984	73.98	2.2179	106.63	3.1968
11	71.96	2.1574	85.93	2.5762	75.96	2.2772	106.63	3.1968
12	75.89	2.2752	87.6	2.6262	81.07	2.4306	118.00	3.5375
13	77.41	2.3206	87.62	2.6268	81.71	2.4495	126.12	3.7809
14	78.96	2.3673	92.42	2.7706	83.34	2.4984	132.09	3.9600
15	80.01	2.3986	94.4	2.8301	85.4	2.5602	132.09	3.9600
16	81.92	2.4560	96.93	2.9057	86.58	2.5956	136.08	4.0797
17	83.23	2.4952	97.03	2.9088	88.49	2.6529	136.08	4.0797
18	83.93	2.5160	99.16	2.9728	91.7	2.7491	138.58	4.1544
19	88.66	2.6579	101.07	3.03	94.85	2.8435	140.26	4.2048
20	92.37	2.7692	109.3	3.2766	95.68	2.8685	140.26	4.2048
21	93.13	2.7918	109.46	3.2815	101.13	3.0319	142.48	4.2715
22	95.75	2.8705	110.08	3.3002	101.76	3.0507	143.62	4.3055
23	96.46	2.8918	111.54	3.3438	103.38	3.0993	143.62	4.3055
24	97.73	2.9298	114.18	3.4232	104.54	3.1339	151.31	4.5361
25	99.53	2.9838	116.63	3.4964	108.19	3.2435	154.65	4.6362
26	102.27	3.0660	118.71	3.5587	114.14	3.4218	154.65	4.6362
27	104.33	3.1278	119.67	3.5877	117.48	3.5221	159.15	4.7712
28	108.69	3.2585	121.01	3.6277	118.82	3.5621	159.36	4.7776
29	111.43	3.3404	125.18	3.7529	120.41	3.6097	159.36	4.7776
30	113.47	3.4018	126.39	3.7891	123.02	3.6882	165.75	4.9692
31	116.07	3.4797	127.49	3.822	125.08	3.7497	165.75	4.9692
32	117.54	3.5236	128.74	3.8596	129.8	3.8913	168.21	5.0429
33	122.65	3.6770	134.16	4.0221	130.71	3.9186	168.21	5.0429
34	125.30	3.7565	138.8	4.1611	131.84	3.9525	174.44	5.2296
35	125.62	3.7661	140.48	4.2116	135.38	4.0585	174.44	5.2296
36	128.78	3.8606	146.92	4.4045	150.38	4.5082	175.07	5.2486
37	147.17	4.4120	147.7	4.4279	152.83	4.5818	176.00	5.2764
38	148.64	4.4561	149.46	4.4808	154.54	4.633	181.73	5.4481
39	150.65	4.5165	152.84	4.582	167.28	5.015	191.96	5.7547
40	158.10	4.7397	157.8	4.7308	169.25	5.074	191.96	5.7547

Table S1 (continued). Phonon vibrations of transition state, initial state, and final state of reaction: NO* ---> N* + O* on the Pt (111) surface

Phonon calculation, Transition state			Phonon calculation, Initial state		Phonon calculation, Final state		Phonon calculation, Pt(111) slab	
mode	[cm^{-1}]	[THz]	[cm^{-1}]	[THz]	[cm^{-1}]	[THz]	[cm^{-1}]	[THz]
41	161.60	4.8447	161.82	4.8513	170.85	5.122	196.17	5.8811
42	168.72	5.0580	165.62	4.9651	173.18	5.1919	196.17	5.8811
43	171.91	5.1538	169.37	5.0776	175.79	5.2702	205.97	6.1749
44	172.84	5.1815	170.16	5.1014	177.37	5.3175	205.97	6.1749
45	175.16	5.2511	176.63	5.2952	178.71	5.3575	208.48	6.2501
46	178.30	5.3454	178.41	5.3487	180.24	5.4035	208.48	6.2501
47	178.75	5.3588	179.36	5.3771	184.59	5.5339	223.15	6.6900
48	179.24	5.3735	180.67	5.4162	186.82	5.6009	223.15	6.6900
49	181.29	5.4351	192.01	5.7564	393.99	11.8117		
50	282.51	8.4694	349.58	10.48	472.68	14.1707		
51	324.85	9.7388	387.69	11.6226	492.5	14.7647		
52	445.43	13.3537	442.39	13.2625	518.35	15.5398		
53	511.78	15.3428	539.17	16.1638	572.05	17.1497		
54	603.31	18.0868	1515.36	45.4293	588.19	17.6335		

Table S2. Phonon vibrations of transition state, initial state, and final state of reaction: NO* ---> N* + O* on the Rh_3Pt (111) surface.

Phonon calculation, Transition state			Phonon calculation, Initial state		Phonon calculation, Final state		Phonon calculation, PtRh(111) slab	
mode	[cm^{-1}]	[THz]	[cm^{-1}]	[THz]	[cm^{-1}]	[THz]	[cm^{-1}]	[THz]
1	-158.31	-4.7460	-0.00	-0.0000	0.00	0.0000	-0.00	-0.0000
2	-0.00	-0.0000	-0.00	-0.0000	0.00	0.0000	0.00	0.0000
3	0.00	0.0000	0.00	0.0000	0.00	0.0000	0.00	0.0000
4	0.00	0.0000	43.46	1.3028	44.92	1.3468	71.09	2.1312
5	24.61	0.7378	44.65	1.3387	46.11	1.3823	98.02	2.9386
6	63.30	1.8977	66.03	1.9795	68.21	2.0448	119.71	3.5889
7	69.68	2.0891	66.43	1.9916	68.61	2.0568	128.07	3.8395
8	71.16	2.1334	86.46	2.5920	88.05	2.6396	141.46	4.2410
9	84.19	2.5241	86.76	2.6009	88.74	2.6604	147.49	4.4216
10	95.22	2.8548	89.56	2.6849	88.94	2.6664	147.97	4.4361
11	97.77	2.9312	92.67	2.7781	96.11	2.8813	150.19	4.5027
12	102.84	3.0831	99.71	2.9891	102.96	3.0865	150.19	4.5027
13	107.83	3.2327	99.71	2.9893	103.32	3.0975	152.69	4.5776
14	112.01	3.3581	104.31	3.1271	112.05	3.3591	154.24	4.6240
15	116.41	3.4900	113.40	3.3997	113.10	3.3907	154.24	4.6240
16	122.26	3.6653	114.07	3.4198	113.24	3.3947	174.62	5.2349
17	124.96	3.7461	116.37	3.4886	117.92	3.5352	175.81	5.2706
18	133.44	4.0005	116.53	3.4935	118.70	3.5585	175.81	5.2706

Table S2 (Continued). Phonon vibrations of transition state, initial state, and final state of reaction: NO* ---> N* + O* on the Rh_3Pt (111) surface.

Phonon calculation, Transition state			Phonon calculation, Initial state		Phonon calculation, Final state		Phonon calculation PtRh(111) slab	
mode	[cm^{-1}]	[THz]	[cm^{-1}]	[THz]	[cm^{-1}]	[THz]	[cm^{-1}]	[THz]
19	136.07	4.0794	121.84	3.6527	119.51	3.5828	178.85	5.3619
20	137.31	4.1166	122.39	3.6693	124.33	3.7274	185.39	5.5578
21	141.13	4.2310	128.74	3.8595	124.49	3.7322	202.53	6.0717
22	143.38	4.2984	130.54	3.9135	128.33	3.8473	202.53	6.0717
23	147.09	4.4096	133.08	3.9895	136.72	4.0988	206.73	6.1977
24	152.56	4.5737	136.75	4.0997	137.45	4.1206	216.15	6.4801
25	152.65	4.5764	137.28	4.1155	138.12	4.1406	220.11	6.5987
26	158.65	4.7561	142.05	4.2585	142.28	4.2655	220.11	6.5987
27	161.19	4.8325	148.06	4.4386	148.23	4.4438	226.18	6.7806
28	166.86	5.0024	148.57	4.4540	148.27	4.4451	245.01	7.3454
29	167.47	5.0205	148.73	4.4590	149.77	4.4899	245.01	7.3454
30	174.90	5.2434	155.07	4.6490	152.25	4.5644	246.77	7.3981
31	183.73	5.5080	155.30	4.6557	152.43	4.5698	256.05	7.6762
32	186.79	5.5997	164.16	4.9213	166.90	5.0035	256.05	7.6762
33	188.52	5.6518	164.22	4.9230	178.95	5.3649	262.42	7.8671
34	190.33	5.7060	170.98	5.1260	179.18	5.3716	262.42	7.8671
35	195.10	5.8489	171.18	5.1320	181.61	5.4446	289.09	8.6667
36	202.22	6.0623	171.90	5.1534	185.76	5.5691	289.09	8.6667
37	206.56	6.1926	178.19	5.3419	188.40	5.6482	291.43	8.7367
38	209.11	6.2690	183.32	5.4959	188.44	5.6492	291.43	8.7367
39	210.70	6.3166	185.14	5.5504	198.28	5.9441	294.70	8.8349
40	211.80	6.3496	185.38	5.5574	209.60	6.2838	294.70	8.8349
41	213.51	6.4009	187.78	5.6294	214.73	6.4373	300.89	9.0204
42	219.87	6.5915	196.49	5.8905	215.08	6.4479	300.89	9.0204
43	221.68	6.6457	196.66	5.8958	220.57	6.6125	312.12	9.3572
44	224.92	6.7428	210.04	6.2970	224.91	6.7427	312.12	9.3572
45	225.45	6.7589	213.44	6.3987	226.57	6.7924	345.37	10.3540
46	234.13	7.0191	213.52	6.4011	226.69	6.7960	345.37	10.3540
47	243.82	7.3097	217.68	6.5257	232.10	6.9582	356.30	10.6816
48	252.85	7.5802	220.18	6.6008	232.22	6.9617	356.30	10.6816
49	254.62	7.6333	226.34	6.7854	433.50	12.9959		
50	267.29	8.0133	226.52	6.7908	435.49	13.0556		
51	281.69	8.4448	357.57	10.7196	499.61	14.9779		
52	471.05	14.1216	358.58	10.7501	520.78	15.6126		
53	520.37	15.6004	368.25	11.0397	520.85	15.6148		
54	928.90	27.8478	1512.99	45.3582	563.19	16.8841		