Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for:

Synergistically engineering of shell thickness and core ordering to boost the oxygen reduction performance

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Coordinate files of $L1_0$, $L1_1$, $L1_2$ and $L1_3$ ordered phases(*.vasp file).

$L1_0$ phase:

L10.vasp

1.0

7.9539999962	**0.0000000000**	**0.0000000000**
0.0000000000	**7.9539999962**	**0.0000000000**
0.0000000000	**0.0000000000**	**7.9539999962**

Pt	**TM**
16	**16**

Direct

0.000000000	**0.000000000**	**0.000000000**
0.250000000	**0.250000000**	**0.000000000**
0.500000000	**0.000000000**	**0.000000000**
0.750000000	**0.250000000**	**0.000000000**
0.000000000	**0.500000000**	**0.000000000**
0.250000000	**0.750000000**	**0.000000000**
0.500000000	**0.500000000**	**0.000000000**
0.750000000	**0.750000000**	**0.000000000**
0.000000000	**0.000000000**	**0.500000000**
0.250000000	**0.250000000**	**0.500000000**
0.500000000	**0.000000000**	**0.500000000**
0.750000000	**0.250000000**	**0.500000000**
0.000000000	**0.500000000**	**0.500000000**
0.250000000	**0.750000000**	**0.500000000**
0.500000000	**0.500000000**	**0.500000000**
0.750000000	**0.750000000**	**0.500000000**
0.000000000	**0.250000000**	**0.250000000**
0.250000000	**0.000000000**	**0.250000000**
0.500000000	**0.250000000**	**0.250000000**
0.750000000	**0.000000000**	**0.250000000**
0.000000000	**0.750000000**	**0.250000000**
0.250000000	**0.500000000**	**0.250000000**
0.500000000	**0.750000000**	**0.250000000**
0.750000000	**0.500000000**	**0.250000000**
0.000000000	**0.250000000**	**0.750000000**
0.250000000	**0.000000000**	**0.750000000**
0.500000000	**0.250000000**	**0.750000000**
0.750000000	**0.000000000**	**0.750000000**
0.000000000	**0.750000000**	**0.750000000**
0.250000000	**0.500000000**	**0.750000000**
0.500000000	**0.750000000**	**0.750000000**
0.750000000	**0.500000000**	**0.750000000**

$L1_1$ phase:

L11.vasp

1.0

7.9539999962	**0.0000000000**	**0.0000000000**
0.0000000000	**7.9539999962**	**0.0000000000**
0.0000000000	**0.0000000000**	**7.9539999962**

Pt	**TM**
16	**16**

Direct

0.000000000	**0.000000000**	**0.000000000**
0.500000000	**0.250000000**	**0.250000000**
0.750000000	**0.000000000**	**0.250000000**
0.750000000	**0.250000000**	**0.000000000**
0.000000000	**0.750000000**	**0.250000000**
0.250000000	**0.500000000**	**0.250000000**
0.250000000	**0.750000000**	**0.000000000**
0.500000000	**0.500000000**	**0.000000000**
0.000000000	**0.250000000**	**0.750000000**
0.250000000	**0.000000000**	**0.750000000**
0.250000000	**0.250000000**	**0.500000000**
0.500000000	**0.000000000**	**0.500000000**
0.000000000	**0.500000000**	**0.500000000**
0.500000000	**0.750000000**	**0.750000000**
0.750000000	**0.500000000**	**0.750000000**
0.750000000	**0.750000000**	**0.500000000**
0.000000000	**0.250000000**	**0.250000000**
0.250000000	**0.000000000**	**0.250000000**
0.250000000	**0.250000000**	**0.000000000**
0.500000000	**0.000000000**	**0.000000000**
0.000000000	**0.500000000**	**0.000000000**
0.500000000	**0.750000000**	**0.250000000**
0.750000000	**0.500000000**	**0.250000000**
0.750000000	**0.750000000**	**0.000000000**
0.000000000	**0.000000000**	**0.500000000**
0.500000000	**0.250000000**	**0.750000000**
0.750000000	**0.000000000**	**0.750000000**
0.750000000	**0.250000000**	**0.500000000**
0.000000000	**0.750000000**	**0.750000000**
0.250000000	**0.500000000**	**0.750000000**
0.250000000	**0.750000000**	**0.500000000**
0.500000000	**0.500000000**	**0.500000000**

$L1_2$ phase:

L12-Pt rich(Pt poor).vasp

1.0

7.9539999962	**0.0000000000**	**0.0000000000**
0.0000000000	**7.9539999962**	**0.0000000000**
0.0000000000	**0.0000000000**	**7.9539999962**

Pt(TM)	**TM(Pt)**
24	**8**

Direct

0.000000000	**0.000000000**	**0.000000000**
0.250000000	**0.250000000**	**0.000000000**
0.000000000	**0.250000000**	**0.250000000**
0.500000000	**0.000000000**	**0.000000000**
0.750000000	**0.250000000**	**0.000000000**
0.500000000	**0.250000000**	**0.250000000**
0.000000000	**0.500000000**	**0.000000000**
0.250000000	**0.750000000**	**0.000000000**
0.000000000	**0.750000000**	**0.250000000**
0.500000000	**0.500000000**	**0.000000000**
0.750000000	**0.750000000**	**0.000000000**
0.500000000	**0.750000000**	**0.250000000**
0.000000000	**0.000000000**	**0.500000000**
0.250000000	**0.250000000**	**0.500000000**
0.000000000	**0.250000000**	**0.750000000**
0.500000000	**0.000000000**	**0.500000000**
0.750000000	**0.250000000**	**0.500000000**
0.500000000	**0.250000000**	**0.750000000**
0.000000000	**0.500000000**	**0.500000000**
0.250000000	**0.750000000**	**0.500000000**
0.000000000	**0.750000000**	**0.750000000**
0.500000000	**0.500000000**	**0.500000000**
0.750000000	**0.750000000**	**0.500000000**
0.500000000	**0.750000000**	**0.750000000**
0.250000000	**0.000000000**	**0.250000000**
0.750000000	**0.000000000**	**0.250000000**
0.250000000	**0.500000000**	**0.250000000**
0.750000000	**0.500000000**	**0.250000000**
0.250000000	**0.000000000**	**0.750000000**
0.750000000	**0.000000000**	**0.750000000**
0.250000000	**0.500000000**	**0.750000000**
0.750000000	**0.500000000**	**0.750000000**

$L1_3$ phase:

L13-Pt rich(Pt poor).vasp

1.0

7.9539999962	**0.0000000000**	**0.0000000000**
0.0000000000	**7.9539999962**	**0.0000000000**
0.0000000000	**0.0000000000**	**7.9539999962**

Pt(TM) TM(Pt)

24 8

Direct

0.000000000	**0.000000000**	**0.000000000**
0.000000000	**0.250000000**	**0.250000000**
0.250000000	**0.000000000**	**0.250000000**
0.500000000	**0.250000000**	**0.250000000**
0.750000000	**0.000000000**	**0.250000000**
0.750000000	**0.250000000**	**0.000000000**
0.000000000	**0.750000000**	**0.250000000**
0.250000000	**0.500000000**	**0.250000000**
0.250000000	**0.750000000**	**0.000000000**
0.500000000	**0.500000000**	**0.000000000**
0.500000000	**0.750000000**	**0.250000000**
0.750000000	**0.500000000**	**0.250000000**
0.000000000	**0.250000000**	**0.750000000**
0.250000000	**0.000000000**	**0.750000000**
0.250000000	**0.250000000**	**0.500000000**
0.500000000	**0.000000000**	**0.500000000**
0.500000000	**0.250000000**	**0.750000000**
0.750000000	**0.000000000**	**0.750000000**
0.000000000	**0.500000000**	**0.500000000**
0.000000000	**0.750000000**	**0.750000000**
0.250000000	**0.500000000**	**0.750000000**
0.500000000	**0.750000000**	**0.750000000**
0.750000000	**0.500000000**	**0.750000000**
0.750000000	**0.750000000**	**0.500000000**
0.250000000	**0.250000000**	**0.000000000**
0.500000000	**0.000000000**	**0.000000000**
0.000000000	**0.500000000**	**0.000000000**
0.750000000	**0.750000000**	**0.000000000**
0.000000000	**0.000000000**	**0.500000000**
0.750000000	**0.250000000**	**0.500000000**
0.250000000	**0.750000000**	**0.500000000**
0.500000000	**0.500000000**	**0.500000000**

Table S1 The structural parameters of PtTM alloys

metal	Pt : TM = 1 : 1	
	$L1_0$*	$L1_1$*
Fe	a=b=3.87; c=3.77 (-2.69%)	a=b=c=3.94 (-0.93%)
	α=β=γ=90°	α=β=γ=90.7°
Co	a=b=3.82; c=3.73 (-3.95%)	a=b=c=3.80 (-4.45%)
	α=β=γ=90°	α=β=γ=91.0°
Ni	a=b=3.85; c=3.64 (-3.19%)	a=b=c=3.80 (-4.45%)
	α=β=γ=90°	α=β=γ=91.7°
V	a=b=3.83; c=3.92 (-3.70%)	a=b=c=3.88 (-2.44%)
	α=β=γ=90°	α=β=γ=90.1°
Cu	a=b=3.93; c=3.63 (-1.18%)	a=b=c=3.84 (-3.44%)
	α=β=γ=90°	α=β=γ=91.7°
Ag	a=b=3.95; c=4.29 (-0.68%)	a=b=c=4.05 (1.84%)
	α=β=γ=90°	α=β=γ=88.8°
Pd	a=b=3.98; c=3.93 (-0.08%)	a=b=c=3.96 (-0.43%)
	α=β=γ=90°	α=β=γ=89.7°

*The unit of lattice constants is Ångstrom.

Table S2 The structural parameters of Pt_3M alloys

metal	Pt : TM = 3 : 1	
	$L1_2$*	$L1_3$*
Fe	a=b=c=3.77 (-5.20%)	a=b=c=3.92 (-1.43%)
	α=β=γ=90°	α=β=90°; γ=89.6°
Co	a=b=c=3.89 (-2.19%)	a=b=c=3.90 (-1.94%)
	α=β=γ=90°	α=β=90°; γ=89.6°
Ni	a=b=c=3.89 (-2.19%)	a=b=3.90; c=3.86 (-1.94%)
	α=β=γ=90°	α=β=90°; γ=89.4°
V	a=b=c=3.92 (-1.43%)	a=b=3.92; c=3.93 (-1.43%)
	α=β=γ=90°	α=β=90°; γ=89.2°
Cu	a=b=c=3.91 (-1.68%)	a=b=3.90; c=3.91 (-1.94%)
	α=β=γ=90°	α=β=90°; γ=89.6°
Ag	a=b=c=4.01 (0.83%)	a=b=3.98; c=4.07 (0.08%)
	α=β=γ=90°	α=β=90°; γ=90.5°
Pd	a=b=c=3.97 (-0.18%)	a=b=3.97; c=3.96 (-0.18%)
	α=β=γ=90°	α=β=90°; γ=90.2°

*The unit of lattice constants is Ångstrom.

Table S3 The structural parameters of PtM_3 alloy

metal	Pt : TM = 1 : 3	
	$L1_2$*	$L1_3$*
Fe	a=b=c=3.74 (-5.96%) α=β=γ=90°	a=b=3.75; c=3.74 (-5.71%) α=β=90°; γ=89.1°
Co	a=b=c=3.67 (-7.72%) α=β=γ=90°	a=b=3.65; c=3.58 (-8.22%) α=β=90°;γ=89.6°
Ni	a=b=c=3.66 (-7.97%) α=β=γ=90°	a=b=3.71; c=3.57 (-6.71%) α=β=90°; γ=88.3°
V	a=b=c=3.84 (-3.44%) α=β=γ=90°	a=b=3.78; c=3.96 (-4.95%) α=β=90°; γ=91.2°
Cu	a=b=c=3.74 (-5.96%) α=β=γ=90°	a=b=3.83; c=3.59 (-3.70%) α=β=90°; γ=88.0°
Ag	a=b=c=4.10 (3.09%) α=β=γ=90°	a=b=c=4.10 (3.09%) α=β=γ=90°
Pd	a=b=c=3.96 (-0.43%) α=β=γ=90°	a=b=c=3.96 (-0.43%) α=β=γ=90°

*The unit of lattice constants is Ångstrom.

Table S4 The ΔU_{diss}, f_i and ΔE_i of $L1_0$–PtTM/Pt_{nL} slabs

Type of order phase	metals	n	ΔU_{diss} (V)	f_i	ΔE_i (eV)
$L1_0$	Fe	1	0.282	0.5	0.250
			0.192	0.5	0.220
		2	0.064	0.5	0.027
			-0.002	0.5	0.043
		3	-0.031	0.5	-0.010
			-0.003	0.5	0.050
		4	-0.028	0.5	0.033
			-0.028	0.5	0.033
	Co	1	0.198	0.5	0.277
			0.088	0.5	0.201
		2	-0.009	0.5	0.081
			-0.065	0.5	0.049
		3	-0.087	0.5	0.027
			-0.068	0.5	0.073
		4	-0.100	0.5	0.022
			-0.100	0.5	0.022
	Ni	1	0.123	0.5	0.136
			0.015	0.5	0.303
		2	-0.099	0.5	0.099
			-0.045	0.5	0.040
		3	-0.107	0.5	0.027
			-0.121	0.5	0.056
		4	-0.144	0.5	-0.012
			-0.144	0.5	-0.012
	V	1	0.347	0.5	0.182
			0.252	0.5	0.340
		2	0.110	0.5	0.011
			0.136	0.5	0.236
		3	-0.042	0.5	-0.117
			0.016	0.5	-0.007
		4	0.009	0.5	0.035
			0.009	0.5	0.035

Table S5 The ΔU_{diss}, f_i and ΔE_i of $L1_1$−PtTM/Pt_{nL} slabs

Type of order phase	metals	n	ΔU_{diss} (V)	f_i	ΔE_i (eV)
$L1_1$	Cu	1	0.334	1	0.412
		2	0.021	1	-0.058
		3	0.055	1	0.051
		4	0.030	1	0.023
	Ag	1	0.125	1	0.287
		2	-0.113	1	-0.209
		3	-0.020	1	-0.066
		4	-0.012	1	-0.049
	Pd	1	0.123	1	-0.010
		2	0.039	1	0.001
		3	0.026	1	-0.040
		4	0.026	1	-0.009

Table S6 The ΔU_{diss}, f_i and ΔE_i of $L1_2$−Pt_3TM/Pt_{nL} slabs

Type of order phase	metals	n	ΔU_{diss} (V)	f_i	ΔE_i (eV)
$L1_2$	Fe	1	0.219	0.75	0.120
			0.090	0.25	0.051
		2	0.075	0.75	0.004
			0.019	0.25	0.003
		3	0.041	0.75	-0.001
			0.073	0.25	0.045
		4	0.034	0.75	0.009
			0.034	0.25	0.009
	Co	1	0.195	0.75	0.124
			0.081	0.25	0.064
		2	0.069	0.75	0.021
			0.022	0.25	0.034
		3	0.041	0.75	0.023
			0.058	0.25	0.043
		4	0.030	0.75	0.021
			0.030	0.25	0.021
	V	1	0.231	0.75	0.053
			0.016	0.25	0.206
		2	0.083	0.75	0.006
			0.103	0.25	0.171
		3	0.036	0.75	-0.016
			0.065	0.25	0.032
		4	0.034	0.75	0.009
			0.034	0.25	0.009

Table S7 The ΔU_{diss}, f_i and ΔE_i of $L1_3$−Pt_3TM/Pt_{nL} slabs

Type of order phase	metals	n	ΔU_{diss} (V)	f_i	ΔE_i (eV)
$L1_3$	Ni	1	0.214	0.5	0.130
			0.136	0.5	0.046
		2	0.122	0.5	0.089
			0.031	0.5	-0.003
		3	0.046	0.5	0.023
			0.058	0.5	0.036
		4	0.028	0.5	0.018
			0.028	0.5	0.018
	Cu	1	0.232	0.5	0.186
			0.220	0.5	0.056
		2	-0.004	0.5	-0.108
			0.163	0.5	0.103
		3	0.038	0.5	0.000
			0.049	0.5	-0.013
		4	0.035	0.5	0.011
			0.035	0.5	0.011
	Ag	1	0.232	0.5	0.042
			0.220	0.5	-0.049
		2	-0.004	0.5	-0.199
			0.163	0.5	0.001
		3	0.038	0.5	-0.079
			0.049	0.5	-0.100
		4	0.035	0.5	-0.052
			0.035	0.5	-0.052
	Pd	1	0.062	0.5	-0.012
			0.096	0.5	-0.007
		2	0.061	0.5	0.014
			0.000	0.5	-0.043
		3	0.016	0.5	-0.033
			0.024	0.5	-0.033
		4	0.015	0.5	-0.034
			0.015	0.5	-0.034

Table S8 The ΔU_{diss}, f_i and ΔE_i of $L1_2$−$PtTM_3/Pt_{nL}$ slabs

Type of order phase	metals	n	ΔU_{diss} (V)	f_i	ΔE_i (eV)
$L1_2$	Fe	1	0.122	0.25	0.415
			0.212	0.75	0.401
		2	-0.103	0.25	0.097
			-0.060	0.75	0.028
		3	-0.201	0.25	-0.300
			-0.225	0.75	-0.064
		4	-0.223	0.25	-0.093
			-0.223	0.75	-0.093
	V	1	0.113	0.25	-0.221
			0.415	0.75	-0.009
		2	0.146	0.25	0.264
			0.101	0.75	-0.106
		3	-0.009	0.25	-0.013
			-0.059	0.75	-0.126
		4	-0.010	0.25	0.036
			-0.010	0.75	0.036
	Cu	1	0.071	0.25	0.209
			0.022	0.75	0.396
		2	-0.209	0.25	-0.052
			-0.058	0.75	0.144
		3	-0.187	0.25	-0.140
			-0.195	0.75	0.046
		4	-0.239	0.25	-0.193
			-0.239	0.75	-0.193

Table S9 The ΔU_{diss}, f_i and ΔE_{ads} of $L1_3$–$PtTM_3/Pt_{nL}$ slabs

Type of order phase	metals	n	ΔU_{diss} (V)	f_i	ΔE_i (eV)
$L1_3$	Ag	1	-0.052	0.5	-0.224
			-0.248	0.5	-0.526
		2	-0.296	0.5	-0.314
			-0.318	0.5	-0.317
		3	-0.181	0.5	-0.208
			-0.193	0.5	-0.193
		4	-0.148	0.5	-0.134
			-0.148	0.5	-0.134
	Pd	1	0.094	0.5	-0.002
			0.061	0.5	-0.006
		2	0.040	0.5	-0.010
			0.029	0.5	-0.013
		3	0.030	0.5	-0.020
			0.023	0.5	-0.022
		4	0.025	0.5	-0.013
			0.025	0.5	-0.013

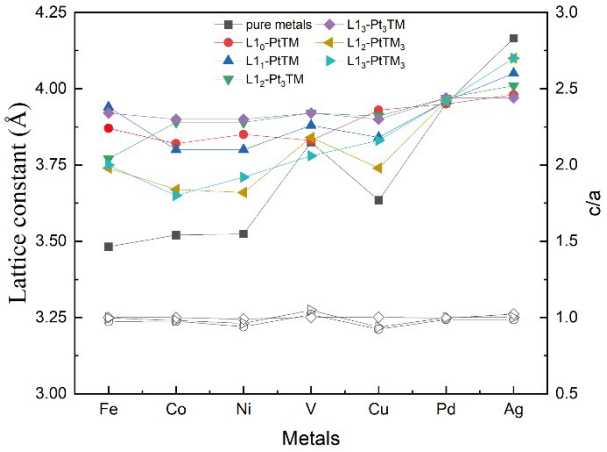

Figure S1 The lattice constants of different metals and alloys assumed as FCC phase