Supporting Information for Face-Centered Tetragonal (FCT) Fe and Co alloys of Pt as catalysts for oxygen reduction reaction(ORR) : A DFT study

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1 Anisotropic contraction

In the manuscript, we show that $L1_0$-CoPt/Pt experiences an in-plane biaxial strain of -4.50% along $[0\bar{1}1]$ and -4.25% along $[\bar{1}10]$ with respect to unstrained Pt. On the other hand, $L1_0$-FePt/Pt experiences a strain of -3.47% and -2.23% along $[0\bar{1}1]$ and $[\bar{1}10]$ respectively. The different strain level along $[0\bar{1}1]$ and $[\bar{1}10]$ is attributed to the anisotropic contraction of unstrained fcc Pt to fct structures as shown in Figure S1.
The procedure used to determine the anisotropic contraction is:

1. Construct fcc Pt bulk using ASE and optimize the lattice constants to obtain the unstrained "a","b" and "c" orthogonal lattice vectors as showin in Figure S1(a) (Here, "a" = "b" = "c").

2. Replace required Pt to Fe to form $L1_0$-FePt bulk. We optimize the lattice constants to obtain compressively strained orthogonal vectors, "$\bar{a}$","$\bar{b}$" and "$\bar{c}$" (Here, "$\bar{a}$" = "$\bar{b}$" $\neq$ "$\bar{c}$").

We observe that the change (contraction) in the three orthogonal directions ("a", "b" and "c") are different (The "c" direction gets contracted with a slightly higher % than "a" and "b").

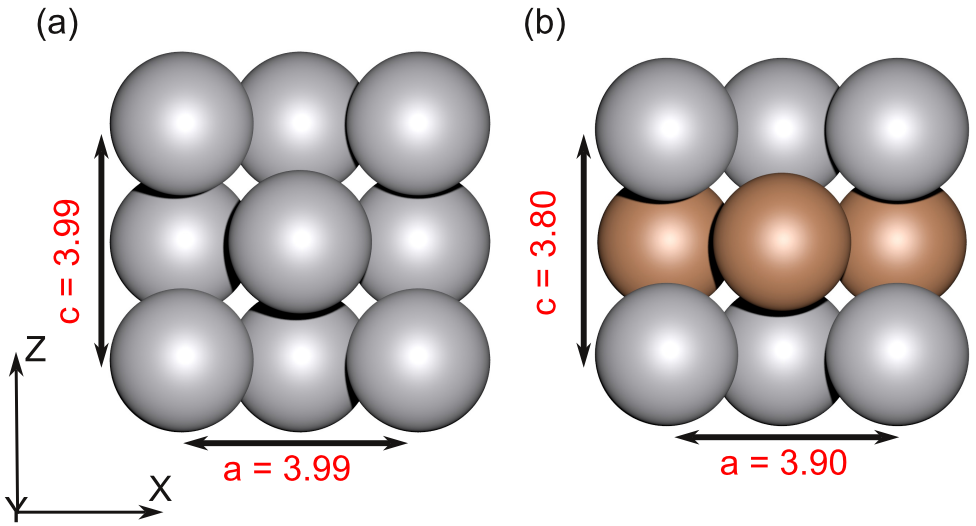

Figure S1: Lattice constants showing anisotropic contraction of (a) unstrained fcc Pt bulk to (b) $L1_0$-FePt bulk. The distances are in Angstroms($\AA$)

2 Binding sites for the ORR intermediates

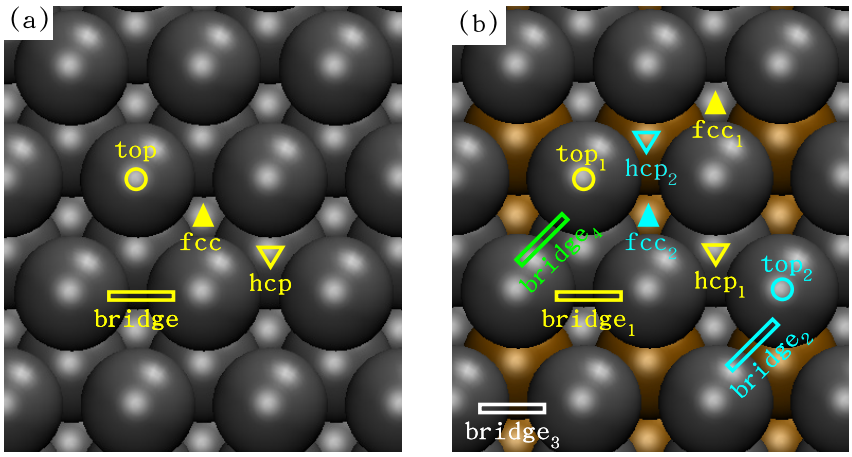

Figure S2: Plausible unique adsorption sites on (a) unstrained fcc Pt (111) surface (similar to $L1_0$-MPt/Pt_n(111) surfaces for n=2, 3 or 4) versus (b) $L1_0$-MPt/Pt_1(111) surface

Table S1: Calculated potential energy, E_{pot} for stable adsorption sites on $L1_0$-FePt/Pt_1(111) surface

Adsorbate	Stable Adsorption Site(s)	E_{pot} (eV)
O_2*	$bridge_2$	-332.359
O*	fcc_1	-328.649
	fcc_2	-328.334
	hcp_1	-328.307
	hcp_2	-328.308
HO*	top_1	-332.743
	top_2	-332.758
	$bridge_3$	-332.537
HOO*	top_1	-336.249
	top_2	-336.257

Table S2: Calculated potential energy, E_{pot} for stable adsorption sites on $L1_0$-CoPt/Pt_1(111) surface

Adsorbate	Stable Adsorption Site(s)	E_{pot} (eV)
O_2*	$bridge_1$	-309.536
	$bridge_2$	-309.588
	$bridge_4$	-309.559
O*	fcc_1	-305.798
	fcc_2	-305.625
	hcp_1	-305.517
	hcp_2	-305.518
HO*	top_1	-309.959
	top_2	-309.999
	$bridge_2$	-309.863
	$bridge_3$	-309.827
HOO*	top_1	-313.441
	top_2	-313.459

3 Alternative pathway to form water

Here, we study the disproportionation reaction of two HO* reacting to form H_2O and O*. Figure S3 shows the free energy landscape for the dissociative mechanism through the disproportionation reaction. We observe that the uphill change in free enregy of the two potential dependent steps D_2° and D_3° are equal since they pertain to the same reaction - protonation of O* to HO*. We assume low coverages for simplicity *i.e.* 2HO* represents two times the energy of HO* calculated separately. Tables S3 & S4 shows the change in free energy associated with each steps invloved in the alternate pathway. Here, the "alternate pathway" denotes the route having formation of water via the disproportion reaction instead of protonation of HO* to H_2O. The energy required for the alternate pathway free energy landscape to be completely downhill (ΔG°) is given as the change in uphill free energy of the potential limiting step (D_2° or D_3°) plus the free energy required for the disproportionation reaction (D_4°). The step D_4° is potential independent but rather depends on the temperature. We observe that although ΔG° for alternate pathway and overpotential, η for the original dissociative pathway are similar (See Tables S3 & S4), the former is predicted to have much lower rate at low temperatures around 300 K due to significant thermodynamic barrier of the step D_4° (low rate at low temperatures) except for unstrained fcc Pt which has an uphill change in free energy of only 0.06 eV.

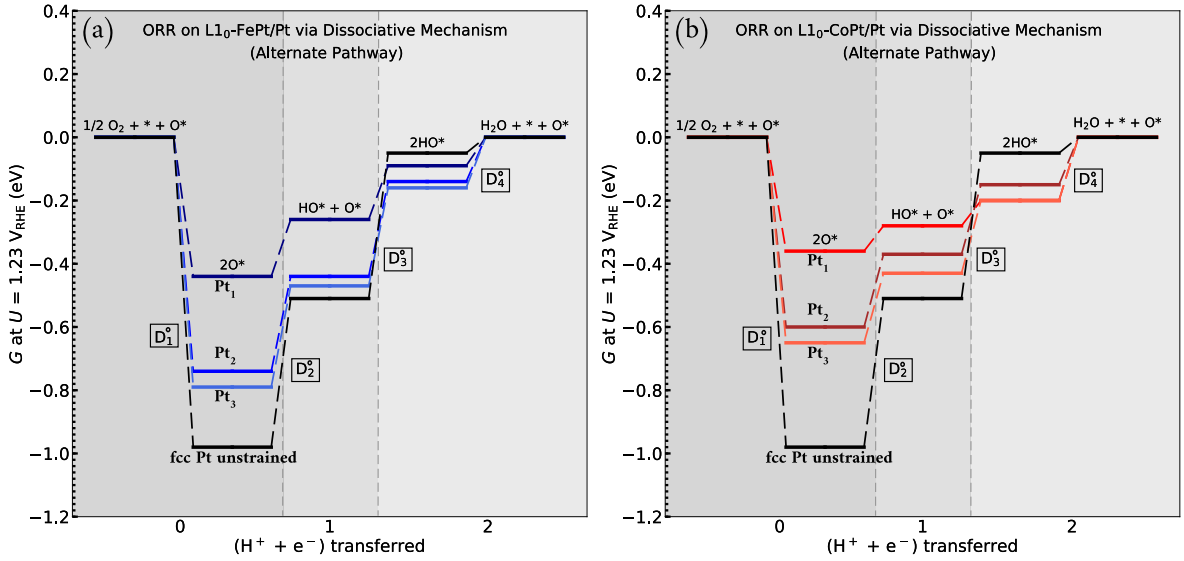

Figure S3: Free energy diagrams at $U = 1.23$ V for oxygen reduction reactions via dissociative mechanism through disproprtionation reaction on (a) L1$_0$-FePt/Pt$_n$ and (b) L1$_0$-CoPt/Pt$_n$ where (n = 1,2,3).

Table S3: Comparison between calculated change in free energies for the steps in dissociative mechanism via alternate and original pathway over L1$_0$-FePt and unstrained fcc Pt. Here, η denotes the overpotential via the original dissociative pathway and ΔG° denotes the required free energy for the alternate dissociative pathway to be become downhill.

System	D_1° (eV)	D_2° (eV)	D_3° (eV)	D_4° (eV)	ΔG° (eV)	η (eV)
L1$_0$-FePt/Pt$_1$	-0.44	0.17	0.17	0.10	0.27	0.26
L1$_0$-FePt/Pt$_2$	-0.74	0.30	0.30	0.14	0.44	0.44
L1$_0$-FePt/Pt$_3$	-0.79	0.32	0.32	0.15	0.47	0.47
L1$_0$-FePt/Pt$_4$	-0.73	0.26	0.26	0.21	0.47	0.47
fcc Pt (unstrained)	-0.98	0.46	0.46	0.06	0.52	0.51

Table S4: Comparison between calculated change in free energies for the steps in dissociative mechanism via alternate and original pathway over $L1_0$-CoPt and unstrained fcc Pt. Here, η denotes the overpotential via the original dissociative pathway and ΔG° denotes the required free energy for the alternate dissociative pathway to be become downhill.

System	D_1° (eV)	D_2° (eV)	D_3° (eV)	D_4° (eV)	ΔG° (eV)	η (eV)
$L1_0$-CoPt/Pt_1	-0.36	0.08	0.08	0.20	0.28	0.28
$L1_0$-CoPt/Pt_2	-0.60	0.23	0.23	0.15	0.38	0.37
$L1_0$-CoPt/Pt_3	-0.65	0.22	0.22	0.20	0.44	0.43
$L1_0$-CoPt/Pt_4	-0.63	0.20	0.20	0.23	0.44	0.43
fcc Pt (unstrained)	-0.98	0.46	0.46	0.06	0.52	0.51

4 Eigenforces and Positions

As supporting information, we also include the values of the eigenforces on each atom (in units of eV/Å) and positions of each optimized structure (in units of Å). The geometry and eigenforce (if existing) for a model system are given as a python dictionary. The key describes the model system and the value is also a dictionary comprising the geometry as an ASE Atoms object (and the eigenforce for model systems without strain). For example, the key 'Pt111-O-(0.00,0.00)' is paired with the geometry of O adsorbed on Pt(111) surface without strain. It should be noted that in order to obtain the eigenforce, we fixed the surfaces while allowing the adsorbate to relax, as shown by the constraint attribute of the Atoms objects.

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from ase.constraints import FixAtoms

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        'fct Pt111-(-4.50, -4.25), strained as CoPt':
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            34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47])),        },

     'fct Pt111-(-3.47, -2.23), strained as FePt':
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573 }
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