#### Evaluating acid and metallic site proximity in $Pt/\gamma$ -Al<sub>2</sub>O<sub>3</sub>-Cl bifunctional

#### catalysts through an atomic scale geometrical model

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# 1. (S)TEM study of the experimental catalysts



Figure S1. TEM images of a) P-egg and b) T-flat aluminas. From ref. <sup>1</sup> with permission.

#### a) 0.3%Pt/P-egg-0.1%Cl reduced



**Figure S2.** HR-HAADF-STEM images and nanoparticle size histograms of four reduced catalysts a) 0.3%Pt/P-egg-0.1%Cl, b) 1%Pt/P-egg-0.1%Cl, c) 0.3%Cl/T-flat0-0.1%Cl, d) 1%Pt/T-flat-0.1%Cl. White arrows highlight single atoms.

#### a) 0.3%Pt/P-egg-1.4%Cl reduced



**Figure S3**. HR-HAADF-STEM images and nanoparticle size histograms of four reduced catalysts a) 0.3%Pt/P-egg-1.4%Cl, b) 1%Pt/P-egg-1.4%Cl, c) 0.3%Pt/T-flat-1.4%Cl, d) 1%Pt/T-flat-1.4%Cl. White arrows highlight single atoms. Figures c) and d) are from ref<sup>2</sup> (with permission).

Sample	#measured NPS	Average NP size (nm)	Standard deviation (nm)	%[0.6; 1.2]nm
0.3%Pt/P-egg-1.4%Cl	204	0.87	0.19	72
0.3%Pt/ P-egg -0.1%Cl	171	0.87	0.16	75
1%Pt/ P-egg -1.4%Cl	214	0.91	0.18	69
1%Pt/ P-egg -0.1%Cl	205	0.86	0.15	76
0.3%Pt/T-flat-1.4%Cl	202	0.86	0.16	74
0.3%Pt/ T-flat -0.1%Cl	207	0.93	0.16	70
1%Pt/ T-flat -1.4%Cl	242	0.86	0.15	75
1%Pt/ T-flat -0.1%Cl	215	0.88	0.17	73

Table S1. Detailed results of nanoparticle size study, complementary to histograms of Figures S2-S3

Images acquired at higher magnification allow the platinum atoms that compose the nanoparticles to be observed. Nanoparticle morphology was studied measuring HAADF intensity to estimate the number of Pt atoms stacked perpendicular to the electron beam (n) from the intensity of atomic column (I), as the image intensity is roughly proportional to the square of the mean atomic number of the analyzed area (Z).<sup>3</sup> As measurements were performed on thin areas, alumina contribution to intensity can be neglected in first approximation. The intensity of three single atoms was measured, to estimate I<sub>SA</sub> proportional to  $Z_{SA}^2$ . Stating that the atomic number of a column composed of n Pt atoms is equal to  $Z_{SA}$ , by measuring intensity of nanoparticles the *n* parameter can be obtained as  $n \propto VI/I_{SA}$ . At least one NP per sample was studied this way and it was consistently found that the NPs are composed of at most two layers of Pt atoms.

An example is given in Figure S4 for the 1%Pt/P-egg-0.1%Cl sample.



**Figure S4.** Detail of nanoparticle morphological study based on the analysis of the HAADF intensity for 1%Pt/P-egg-0.1%Cl, a) three single atom reference paths, b) path through nanoparticle including five potential "stacks" of atoms, c) intensity graph for path of b) with the calculated n for each "stack".

## 2. Pt and Cl loading of the experimental catalysts

 Table S2. Platinum loading evaluated by XRF and calculated surface coverage of P-egg and T-flat impregnated and calcined materials.

	P-egg - Impregnated + calcined				
	% <sub>w/w</sub> Pt	Pt/nm²			
0.3%Pt/ P-egg	1.37 ± 0.03	1.29 ± 0.07			
1%Pt/ P-egg	$1.41 \pm 0.03$	1.34 ± 0.07			
	T-flat - Impregnated + calcined				
	T-flat - Impregr	ated + calcined			
	T-flat - Impregn % <sub>w/w</sub> Pt	ated + calcined Pt/nm²			
0.3%Pt/ T-flat	T-flat - Impregr % <sub>w/w</sub> Pt 1.18 ± 0.03	hated + calcined Pt/nm <sup>2</sup> 1.37 ± 0.08			

 Table S3. Chlorine loading measured by XRF and calculated surface coverage of oxide and reduced PuralSB3 and TH100 catalysts.

PuralSB3									
	Ox	ide	Reduced						
	% <sub>w/w</sub> Cl	Cl/nm²	% <sub>w/w</sub> Cl	Cl/nm²					
0.3%Pt/PuralSB3-1.4%Cl	$1.50 \pm 0.04$	1.42 ± 0.08	1.25 ± 0.03	$1.18 \pm 0.07$					
0.3%Pt/PuralSB3-0.1%Cl	$0.108 \pm 0.006$	$0.101 \pm 0.008$	0.107 ± 0.006	$0.10 \pm 0.01$					
<b>1%Pt</b> /PuralSB3- <b>1.4%Cl</b>	1.51 ± 0.04	1.44 ± 0.09	1.18 ± 0.03	1.11 ± 0.06					
1%Pt/PuralSB3-0.1%Cl	0.163 ± 0.007	0.15 ± 0.01	0.150 ± 0.007	0.14 ± 0.01					
	Т	H100							
	Ox	ide	Redu	uced					
	% <sub>w/w</sub> Cl	Cl/nm²	% <sub>w/w</sub> Cl	Cl/nm²					
<b>0.3%Pt/</b> TH100- <b>1.4%Cl</b>	1.33 ± 0.03	1.54 ± 0.08	1.08 ± 0.03	1.25 ± 0.07					
<b>0.3%Pt/</b> TH100- <b>0.1%Cl</b>	0.132 ± 0.006	0.15 ± 0.01	0.132 ± 0.006	0.15 ± 0.01					
	1	[							
1%Pt/TH100-1.4%Cl	$1.27 \pm 0.03$	$1.48 \pm 0.08$	$1.02 \pm 0.03$	$1.18 \pm 0.07$					
1%Pt/TH100-0.1%Cl	0.212 ± 0.008	0.24 ± 0.02	$0.214 \pm 0.008$	0.25 ± 0.02					

## 3. Calculated Pt and Cl coverage for model platelets

The calculated Pt and Cl coverage listed in Table 1 is obtained as follows:

$$X/nm^{2}(for n\%_{w/w}X) = \frac{n/MM(X) * N_{A}}{(100 - n) * Calculated specific area}$$

With:

Calculated specific area =  $\frac{Platelet \ surface \ area}{Platelet \ volume \ \ast \ \rho}$ 

MM(X) is the molar mass of the element X. Platelet surface area and volume are calculated from the model platelet dimensions (*a*, *b*,*c* for T-flat and *a* for P-egg) and the density  $\rho$  of gamma-alumina used was of 4 g/cm<sup>3</sup>.

## 4. Pt<sub>13</sub>/edge models described in ref 3

**Table S4.** Optimized Pt13/edge models, configuration A and B, from ref <sup>2</sup> (with permission). The first scheme illustrates the views of the nano-rod that are presented which are as follows: left - top view of the (110) side with Al-side edge facing down and O-side edge facing up; right - side view of the (100) side with edge facing up on the right side. Models color coded white - H; red - O; pink - Al; green - Cl; blue - Pt.



## 5. Polyhedral nets with Pt NP fixed positions

**Table S5.** Polyhedral net of the parallelepiped platelet model of P-egg morphology for all the k and %Cl explored, with fixedPt NP positions considered for distance estimation shown in the white icons. Chlorinated edges are depicted by brokenlines, non-chlorinated edges by full lines. Chlorinated surfaces are depicted by a mesh pattern.









**Table S6.** Polyhedral net of the parallelepiped platelet model of T-flat morphology for all the k and %Cl explored, with fixedPt NP positions considered for distance estimation shown in the white icons. Chlorinated edges are depicted by brokenlines, non-chlorinated edges by full lines. Chlorinated surfaces are depicted by a mesh pattern.







### 6. Estimation of Pt NP-Cl distances

 Table S7. Estimation of Pt NP-Cl distances for P-egg for all k and %Cl considered.

P-egg										
k=1			k=1.5			k=0.5				
1.4%Cl			1.21%Cl			1%Cl				
Pt NP fixed position	Distance PtNP- Cl (nm)	Exposition proportion	Pt NP fixed position	Distance PtNP-Cl (nm)	Exposition proportion	Pt NP fixed position	Distance PtNP-Cl (nm)	Exposition proportion		
Surface Posi	tions		Surface Pos	sitions		Surface Pos	itions			
е	1.23	0.56	е	0.58	0.56	a)	0.70	0.23		
а	1.40	0.28	а	2.09	0.28	b)	0.18	0.14		
с	0.81	0.16	с	1.20	0.16	c)	2.20	0.05		
Surface average distance (nm)	1.21		Surface average distance (nm)	1.10		d)	2.09	0.14		
Edge Positio	ns		Edge Positions			e)	3.48	0.09		
Ø	0.23	0.5	Ø	0.23	0.5	f)	1.90	0.09		
b	0.90	0.25	b	0.9	0.25	g)	2.80	0.09		
d	0.90	0.25	d	0.9	0.25	h)	0.40	0.02		
Edge average distance (nm)	0.68		Edge average distance (nm)	0.57		i)	0.80	0.06		
Global average distance	0.79		Global average distance	0.68		j)	1.92	0.04		
						k)	3.00	0.04		
1.2%Cl edge	saturation		1%Cl			Surface	0.85			

						average distance (nm)		
Pt NP fixed	Distance PtNP-	Exposition	Pt NP fixed	Distance	Exposition	Edge Positio	ns	
			(nm)					
Surface Positions			Surface Pos	sitions		Ø	0.23	0.08
а	1.40	0.84	е	2.09	0.56	l)	0.70	0.25
С	0.80	0.16	а	0.70	0.28	m)	1.39	0.06
Surface average distance (nm)	1.30		с	1.20	0.16	n)	1.56	0.10
Edge Positio	ns		Surface average distance (nm)	1.17		0)	2.78	0.06
Ø	0.23	0.5	Edge Position	ons		p)	4.17	0.02
b	1.40	0.25	Ø	0.23	0.5	q)	2.02	0.04
d	1.40	0.25	b	0.90	0.25	r)	2.87	0.02
Edge average distance (nm)	0.82		d	0.90	0.25	s)	1.56	0.06
Global average	0.92		Edge average	0.57		t)	2.03	0.04
distance			Global average distance	0.70		u)	2.60	0.04
0.5%Cl				1		v)	3.17	0.04
Pt NP fixed	Distance PtNP-	Exposition	0.52%Cl ed	ge saturatio	on	x)	3.48	0.08
Surface Posi	tions	proportion	Pt NP fixed position	Distance PtNP-Cl (nm)	Exposition proportion	y) 2.09 0.		
a)	1.40	0.42	Surface Pos	sitions		Edge average distance (nm)	1.73	
b)	1.98	0.28	а	2.09	0.84	Global average distance	1.54	
c)	4.20	0.09	с	1.20	0.16			
d)	1.98	0.05	Surface average distance (nm)	1.94		4.5%Cl edge	saturati	on
f)	0.81	0.08	Edge Positi	005		Pt NP fixed Distance Exposition position PtNP-Cl proportion		
')		0.00	205010010	0113		position	PtNP-Cl (nm)	proportion
g)	1.62	0.31	Ø	0.23	0.5	Surface Posi	PtNP-CI (nm) tions	proportion
r) g) Surface average distance (nm)	1.62 1.82	0.31	Ø b	0.23	0.5 0.25	Surface Posi	PtNP-CI (nm) tions 0.70	0.84
g) Surface average distance (nm) Edge Positio	1.62 1.82 ns	0.31	Ø b d	0.23 2.09 2.09	0.5	Surface Posi a c	PtNP-CI (nm) tions 0.70 0.40	0.84 0.16
g) Surface average distance (nm) Edge Positio Ø	1.62 1.82 ns 0.23	0.31	Ø b Cd Edge average distance (nm)	0.23 2.09 2.09 1.16	0.5 0.25 0.25	Surface Posi a C Surface average distance (nm)	PtNP-CI (nm) tions 0.70 0.40 0.65	0.84 0.16
r) g) Surface average distance (nm) Edge Positio Ø e)	1.62 1.82 ns 0.23 1.40	0.31	Ø b cl Edge average distance (nm) Global average distance	0.23 2.09 2.09 1.16 1.33	0.5 0.25 0.25	Surface Posi a C Surface average distance (nm) Edge Positio	PtNP-Cl (nm) tions 0.70 0.40 0.65 ns	0.84 0.16
r) g) Surface average distance (nm) Edge Positio Ø e) h)	1.62 1.82 ns 0.23 1.40 2.42	0.31 0.21 0.54 0.08	Ø b cd Edge average distance (nm) Global average distance	0.23 2.09 2.09 1.16 1.33	0.5 0.25 0.25	Surface Posi a C Surface average distance (nm) Edge Positio	PtNP-CI (nm) tions 0.70 0.40 0.65 ns	0.84 0.16 0.23 0.5
r) g) Surface average distance (nm) Edge Positio Ø e) h)	1.62 1.82 ns 0.23 1.40 2.42 2.80	0.31 0.21 0.54 0.08 0.06	Ø b cd Edge average distance (nm) Global average distance	0.23 2.09 2.09 1.16 1.33	0.5	position Surface Posi a C Surface average distance (nm) Edge Positio Ø b	PtNP-Cl (nm) tions 0.70 0.40 0.65 ns 0.70	0.84 0.16 0.23 0.5 0.25
r) g) Surface average distance (nm) Edge Positio Ø e) h) i) j)	1.62 1.82 ns 0.23 1.40 2.42 2.80 3.13	0.00 0.31 0.21 0.54 0.08 0.06 0.10	Ø b cd Edge average distance (nm) Global average distance 0.15%Cl Pt NP fixed position	0.23 2.09 2.09 1.16 1.33 Distance PtNP-Cl (nm)	0.5 0.25 0.25 Exposition	position Surface Posi a C Surface average distance (nm) Edge Positio Ø b d	PtNP-CI (nm) tions 0.70 0.40 0.65 ns 0.70 0.70 0.70	0.84 0.16 0.23 0.5 0.25 0.25
r) g) Surface average distance (nm) Edge Positio Ø e) h) i) j) Edge average distance (nm)	1.62 1.82 ns 0.23 1.40 2.42 2.80 3.13 1.51	0.31 0.21 0.54 0.08 0.06 0.10	Ø b c d Edge average distance (nm) Global average distance 0.15%Cl Pt NP fixed position Surface Pos	0.23 2.09 2.09 1.16 1.33 Distance PtNP-Cl (nm) sitions	0.5 0.25 0.25 Exposition proportion	position Surface Posi a C Surface average distance (nm) Edge Positio Ø b d Edge average distance (nm)	PtNP-CI (nm) tions 0.70 0.40 0.65 ns 0.70 0.70 0.70 0.46	0.84 0.16 0.23 0.25 0.25
<ul> <li>r)</li> <li>g)</li> <li>Surface average distance (nm)</li> <li>Edge Positio</li> <li>Ø</li> <li>e)</li> <li>h)</li> <li>i)</li> <li>j)</li> <li>Edge average distance (nm)</li> <li>Global average distance</li> </ul>	1.62 1.82 ns 0.23 1.40 2.42 2.80 3.13 1.51 1.58	0.00 0.31 0.21 0.54 0.08 0.06 0.10	Ø b cd Edge average distance (nm) Global average distance 0.15%Cl Pt NP fixed position Surface Pos a)	0.23 2.09 2.09 1.16 1.33 Distance PtNP-Cl (nm) sitions 2.09	0.5 0.25 0.25 Exposition proportion	position Surface Posi a C Surface average distance (nm) Edge Positio Ø b d Edge average distance (nm) Global average distance	PtNP-CI (nm) tions 0.70 0.40 0.65 ns 0.70 0.70 0.70 0.70 0.46 0.50	0.84 0.16 0.23 0.5 0.25 0.25
<ul> <li>r)</li> <li>g)</li> <li>Surface average distance (nm)</li> <li>Edge Positio</li> <li>Ø</li> <li>e)</li> <li>h)</li> <li>i)</li> <li>j)</li> <li>Edge average distance (nm)</li> <li>Global average distance</li> </ul>	1.62 1.82 ns 0.23 1.40 2.42 2.80 3.13 1.51 1.58	0.31 0.21 0.54 0.08 0.06 0.10	Ø b cd Edge average distance (nm) Global average distance 0.15%Cl Pt NP fixed position Surface Pos a) b)	0.23 2.09 2.09 1.16 1.33 Distance PtNP-Cl (nm) sitions 2.09 2.95	0.5 0.25 0.25 Exposition proportion	position Surface Posi a C Surface average distance (nm) Edge Positio Ø b d Edge average distance (nm) Global average distance	PtNP-CI (nm) tions 0.70 0.40 0.65 ns 0.70 0.70 0.70 0.70 0.46 0.50	0.84 0.16 0.23 0.5 0.25 0.25
r) g) Surface average distance (nm) Edge Positio Ø e) h) i) j) Edge average distance (nm) Global average distance 0.1%Cl	1.62 1.82 ns 0.23 1.40 2.42 2.80 3.13 1.51 1.58	0.31 0.21 0.54 0.08 0.06 0.10	Ø b c) c)	0.23 2.09 2.09 1.16 1.33 Distance PtNP-Cl (nm) sitions 2.09 2.95 8.60	0.5 0.25 0.25 Exposition proportion	position Surface Posi a C Surface average distance (nm) Edge Positio Ø b d Edge average distance (nm) Global average distance	PtNP-Cl (nm) tions 0.70 0.40 0.65 ns 0.70 0.70 0.70 0.70 0.46 0.50	0.84 0.16 0.23 0.25 0.25
<ul> <li>r)</li> <li>g)</li> <li>Surface average distance (nm)</li> <li>Edge Positio</li> <li>Ø</li> <li>e)</li> <li>h)</li> <li>i)</li> <li>j)</li> <li>Edge average distance (nm)</li> <li>Global average distance</li> <li>0.1%Cl</li> <li>Pt NP fixed position</li> </ul>	1.62 1.82 ns 0.23 1.40 2.42 2.80 3.13 1.51 1.58 Distance PtNP- Cl (nm)	0.00 0.31 0.21 0.54 0.08 0.06 0.10	Ø b classer of our content of the second sec	0.23 2.09 2.09 1.16 1.33 Distance PtNP-Cl (nm) sitions 2.09 2.95 8.60 6.26	0.5 0.25 0.25 Exposition proportion 0.37 0.19 0.09	position Surface Posi a C Surface average distance (nm) Edge Positio Ø b d Edge average distance (nm) Global average distance	PtNP-CI (nm) tions 0.70 0.40 0.65 ns 0.70 0.70 0.70 0.70 0.46 0.50	0.84 0.16 0.23 0.5 0.25 0.25

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f)     3.87     0.02     surface average altisance (nm)     2.57       g)     4.43     0.09     Edge Positum       h)     3.82     0.14     Ø     0.23     0.15       i)     5.64     0.05     j)     2.09     0.42       j)     7.00     0.05     k)     4.17     0.06       k)     9.80     0.05     n)     6.07     0.021       n)     9.80     0.05     n)     6.07     0.021       n)     9.80     0.05     n)     6.07     0.021       n)     9.80     0.05     p)     6.08     0.041       n)     7.14     0.05     p)     6.08     0.041       n)     7.14     0.05     p)     6.08     0.041       surface average datame (nm)     16.21     0.02     r)     6.26     0.08       Surface average datame (nm)     11.62     0.02     r)     6.26     0.08       Surface average datame (nm)     3.02     3.02     3.02     3.02       g)     0.23     0.041     3.02     3.02       g)     0.420     0.023     3.02     3.02       g)     0.420     0.023     3.02       g)	e)	1.89	0.06	i)	5.77	0.04
g)     4.43     0.09     Edge Positum       h)     3.82     0.14     Ø     0.23     0.15       i)     5.64     0.05     j)     2.09     0.42       j)     7.00     0.05     k)     4.17     0.06       k)     9.80     0.15     l)     6.07     0.02       i)     9.80     0.05     n)     4.67     0.17       m)     14.23     0.05     p)     6.08     0.04       o     6.03     0.06     q)     7.52     0.02       p)     16.21     0.02     p)     6.26     0.08       surface average distance (nm)     3.15     distance (nm)     3.15       idstance (nm)     3.13     0.04     0.17       q)     3.13     0.04     0.17       q)     3.13     0.04     0.17       q)     3.13     0.02     3.02       x)     3.50     0.02     0.14       u)     5.77     0.02     0.23       x)     8.52     0.02       x) <td>f)</td> <td>3.87</td> <td>0.02</td> <td>Surface average distance (nm)</td> <td>2.57</td> <td></td>	f)	3.87	0.02	Surface average distance (nm)	2.57	
h)3.820.14Ø0.230.15i)5.640.05j)2.090.42j)7.000.05k)4.170.06k)9.800.05n)4.670.17m)14.230.05o)3.610.04n)7.140.05p)6.080.04o6.030.06q)7.520.02p)16.210.02r)6.260.08surface average distance (nm)3.153.02distance (nm)Edge PositionsGlobal average distance (nm)3.02 $\phi$ 0.230.040.17q)3.130.020.02s)3.130.02r)4.200.02s)3.130.02v)5.600.02x)8.400.02y)2.420.06 $\alpha$ 5.220.02y)2.420.06 $\beta$ 6.480.06y)2.420.06 $\beta$ 6.480.06y)9.800.023)6.760.023)6.760.024)4.200.135)5.050.026)5.600.027)5.770.026)5.600.027)5.770.026)5.600.027)5.770.026)5.600.02	g)	4.43	0.09	Edge Positi	ons	
i)       5.64       0.05       j)       2.09       0.42         j)       7.00       0.05       k)       4.17       0.06         k)       9.80       0.05       n)       4.67       0.17         m)       14.23       0.05       o)       3.61       0.04         n)       7.14       0.05       p)       6.08       0.04         o       6.03       0.06       q)       7.52       0.02         p)       16.21       0.02       r)       6.26       0.08         Surface average distance (nm]       3.15       astrace average distance (nm]       3.02         g/g       0.23       0.04       overage distance (nm]       3.02         g/g       0.23       0.04       overage distance (nm]       3.02         g/g       0.313       0.02       overage distance (nm]       3.02         g/g       0.313       0.02       overage distance (nm]       strace (nm]         g/g       0.313       0.02       overage distance (nm]       strace (nm]         g/g       0.313       0.02       overage distance (nm]       strace (nm]         g/g       0.50       0.02       overage distance (nm] <td>h)</td> <td>3.82</td> <td>0.14</td> <td>Ø</td> <td>0.23</td> <td>0.15</td>	h)	3.82	0.14	Ø	0.23	0.15
j)     7.00     0.05     k)     4.17     0.06       k)     9.80     0.15     I)     6.07     0.02       l)     9.80     0.05     n)     4.67     0.17       m)     14.23     0.05     o)     3.61     0.04       n)     7.14     0.05     p)     6.08     0.04       o     6.03     0.06     q)     7.52     0.02       p)     16.21     0.02     r)     6.26     0.08       Surface distance (nm)     16.21     0.02     r)     6.26     0.08       Surface distance (nm)     16.21     0.02     r)     6.26     0.08       Surface distance (nm)     16.21     0.02     3.15     3.15       Edge Positiv     Sidolal sverage distance (nm)     3.02     3.02       Ø     0.23     0.04     5     5       b)     1.40     0.02     3.13     3.02       r)     4.20     0.02     5     5       s)     3.13     0.04     5       t)     2.80     0.02     5       x)     8.52     0.02     5       x)     8.52     0.02       x)     8.52     0.02    y)	i)	5.64	0.05	j)	2.09	0.42
k)9.800.15I)6.070.02I)9.800.05n)4.670.17m)14.230.05p)6.080.04n7.140.05p)6.080.04o6.030.06q)7.520.02p)16.210.02r)6.260.08Surface average distance (nm)1.10Surface (nm)3.15distance (nm)0.230.04Surface (nm)3.02Ø0.230.04Surface (nm)3.02global3.130.02Surface (nm)3.13global3.130.02Surface (nm)3.15global3.130.02Surface (nm)3.15global3.130.02Surface (nm)Surface (nm)global3.130.02Surface (nm)Surface (nm)global3.130.02Surface (nm)Surface (nm)global3.130.04Surface (nm)Surface (nm)global3.130.04Surface (nm)Surface (nm)global3.130.04Surface (nm)Surface (nm)global3.130.04Surface (nm)Surface (nm)global3.130.04Surface (nm)Surface (nm)global3.130.02Surface (nm)Surface (nm)global3.130.02Surface (nm)Surface (nm)global3.130.02Surface (nm)Surface (nm)glo	j)	7.00	0.05	k)	4.17	0.06
1)         9.80         0.05         n)         4.67         0.17           m)         14.23         0.05         o)         3.61         0.04           n)         7.14         0.05         p)         6.08         0.04           o         6.03         0.06         q)         7.52         0.02           p)         16.21         0.02         r)         6.26         0.08           Surface average distance (nm)         4.91         Edge average distance (nm)         3.15         0.02           Edge Positivitie         Sidobal average distance (nm)         3.02         3.02         0.04           b)         1.40         0.17         3.02         0.04         0.02           g)         3.13         0.002         0.03         0.04         0.02           y)         3.13         0.04         0.02         0.02         0.03         0.04           u)         5.77         0.02         0.04         0.02         0.04         0.04         0.04         0.04         0.04         0.04         0.04         0.04         0.04         0.04         0.04         0.04         0.04         0.04         0.04         0.04         0.04	k)	9.80	0.15	l)	6.07	0.02
m)         14.23         0.05         o)         3.61         0.04           n)         7.14         0.05         p)         6.08         0.04           o         6.03         0.06         q)         7.52         0.02           p)         16.21         0.02         r)         6.26         0.08           Surface average distance (nm)         4.91         Edge average distance (nm)         3.15         0.02           Edge Positiv         Silobal average distance (nm)         3.02         3.02         0.04           b)         1.40         0.17         0.02         0.02         0.02           r)         4.20         0.02         0.02         0.03         0.04           t)         2.80         0.04         0.02         0.02         0.02         0.02         0.02         0.02         0.03         0.04         0.02         0.03         0.02         0.03         0.04         0.02         0.03         0.04         0.04         0.04         0.04         0.02         0.03         0.04         0.04         0.04         0.04         0.04         0.04         0.04         0.04         0.04         0.04         0.04         0.04         0.04 <td>I)</td> <td>9.80</td> <td>0.05</td> <td>n)</td> <td>4.67</td> <td>0.17</td>	I)	9.80	0.05	n)	4.67	0.17
n)         7.14         0.05         p)         6.08         0.04           o         6.03         0.06         q)         7.52         0.02           p)         16.21         0.02         r)         6.26         0.08           surface average distance (nm)         3.15         3.15         3.15           Edge Position         Silobal average distance (nm)         3.02         3.04           Ø         0.23         0.04         0.17           Ø         1.40         0.17         3.13         0.02           r)         4.20         0.02         0.02         0.03           s)         3.13         0.04         0.17         0.02         0.02           s)         3.13         0.04         0.17         0.02         0.02         0.02           s)         3.13         0.04         0.02         0.02         0.03         0.04           u)         5.77         0.02         0.04         0.02         0.04         0.02           x)         8.40         0.06         0.02         0.03         0.06         0.02           y)         2.42         0.06         0.02         0.03         0.02	m)	14.23	0.05	o)	3.61	0.04
ο         6.03         0.06         q)         7.52         0.02           p)         16.21         0.02         r)         6.26         0.08           Surface average distance (nm)         3.15         3.15         3.15           Edge Position         Global average distance (nm)         3.02         3.04           Ø         0.23         0.04         9         3.02           Ø         1.40         0.17         9         3.13         0.02           q)         3.13         0.04         9         9         9         9           1         2.80         0.04         9	n)	7.14	0.05	p)	6.08	0.04
p)         16.21         0.02         r)         6.26         0.08           Surface average distance (nm)         4.91         Edge average distance (nm)         3.15         3.15           Edge Positions         Global average distance (nm)         3.02         3.04           Ø         0.23         0.04         0.17           Ø         1.40         0.17         3.13         0.02           r)         4.20         0.02         0.04         0.17           q)         3.13         0.02         0.04         0.17           q)         3.13         0.04         0.17         0.02         0.02           s)         3.13         0.04         0.02         0.02         0.02         0.02           y)         5.60         0.02         0.02         0.08         0.02         0.08         0.06           µ         3.02         0.06         0.02         0.08         0.02         0.08         0.02           y)         2.42         0.06         0.02         0.03         0.02         0.03         0.02           y)         2.42         0.06         0.02         0.03         0.02         0.03         0.02         0	0	6.03	0.06	q)	7.52	0.02
Surface average distance (nm)         4.91         Edge average distance (nm)         3.15           Edge Positions         Global average distance (nm)         3.02           Ø         0.23         0.04           b)         1.40         0.17           q)         3.13         0.02           r)         4.20         0.02           s)         3.13         0.04           t)         2.80         0.04           u)         5.77         0.02           x)         8.52         0.02           x)         8.52         0.02           w)         8.40         0.02           y)         2.42         0.06           α         5.22         0.06           β         6.48         0.06           γ         7.00         0.08           1)         9.80         0.06           2)         8.03         0.02           3)         6.76         0.02           4)         4.20         0.13           5)         5.05         0.02           6)         5.60         0.02           7)         5.77         0.02           Edge avera	p)	16.21	0.02	r)	6.26	0.08
Edge PositionsGlobal adverage distance (nm)3.02Ø0.230.04b)1.400.17q)3.130.02r)4.200.02s)3.130.04t)2.800.04u)5.770.02v)5.600.02x)8.520.02w)8.400.02z)4.080.02y)2.420.06β6.480.06γ7.000.081)9.800.062)8.030.023)6.760.024)4.200.135)5.050.026)5.600.027)5.770.02Edge average distance (nm)4.65Global average distance (nm)4.65	Surface average distance (nm)	4.91		Edge average distance (nm)	3.15	
Ø0.230.04b)1.400.17q)3.130.02r)4.200.02s)3.130.04t)2.800.04u)5.770.02v)5.600.02x)8.520.02w)8.400.02z)4.080.02y)2.420.06 $\alpha$ 5.220.06β6.480.06γ7.000.081)9.800.023)6.760.024)4.200.135)5.050.026)5.600.027)5.770.02Edge average Gistance (m)4.57Global average Gistance (m)4.65	Edge Positio	ins		Global average distance (nm)	3.02	
b)1.400.17q)3.130.02r)4.200.02s)3.130.04t)2.800.04u)5.770.02v)5.600.02x)8.520.02w)8.400.02z)4.080.02y)2.420.06β6.480.06γ7.000.081)9.800.023)6.760.024)4.200.135)5.050.026)5.600.027)5.770.02Edge average distance (nm)4.57Global average distance (nm)4.65	Ø	0.23	0.04			
q)3.130.02r)4.200.02s)3.130.04t)2.800.04u)5.770.02v)5.600.02x)8.520.02w)8.400.02z)4.080.02y)2.420.06α5.220.06β6.480.06γ7.000.081)9.800.023)6.760.024)4.200.135)5.050.026)5.600.027)5.770.02Edge average distance (nm)4.57Global average distance (nm)4.65	b)	1.40	0.17			
r)4.200.02s)3.130.04t)2.800.04u)5.770.02v)5.600.02x)8.520.02w)8.400.02z)4.080.02y)2.420.06β6.480.06γ7.000.081)9.800.023)6.760.024)4.200.135)5.050.026)5.600.027)5.770.02Edge average distance (nm)4.57Global average distance (nm)4.65	q)	3.13	0.02			
s)3.130.04t)2.800.04u)5.770.02v)5.600.02x)8.520.02w)8.400.02z)4.080.02y)2.420.06α5.220.06β6.480.06γ7.000.081)9.800.023)6.760.024)4.200.135)5.050.026)5.600.027)5.770.02Edge average distance (nm)4.57Global average distance (nm)4.65	r)	4.20	0.02			
t)2.800.04u)5.770.02v)5.600.02x)8.520.02w)8.400.02z)4.080.02y)2.420.06α5.220.06β6.480.06γ7.000.081)9.800.062)8.030.023)6.760.024)4.200.135)5.050.026)5.600.02T)5.770.02Edge average distance (nm)4.57Global average distance (nm)4.65	s)	3.13	0.04			
u)5.770.02v)5.600.02x)8.520.02w)8.400.02z)4.080.02y)2.420.06α5.220.06β6.480.06γ7.000.081)9.800.062)8.030.023)6.760.024)4.200.135)5.050.026)5.600.027)5.770.02Edge average distance (nm)4.57 distance (nm)4.65	t)	2.80	0.04			
v)5.600.02x)8.520.02w)8.400.02z)4.080.02y)2.420.06α5.220.06β6.480.06γ7.000.081)9.800.062)8.030.023)6.760.024)4.200.135)5.050.026)5.600.027)5.770.02Edge average distance (nm)4.65	u)	5.77	0.02			
x)8.520.02w)8.400.02z)4.080.02y)2.420.06α5.220.06β6.480.06γ7.000.081)9.800.062)8.030.023)6.760.024)4.200.135)5.050.026)5.600.027)5.770.02Edge average distance (nm)4.65	v)	5.60	0.02			
w) $8.40$ $0.02$ z) $4.08$ $0.02$ y) $2.42$ $0.06$ $\alpha$ $5.22$ $0.06$ $\beta$ $6.48$ $0.06$ $\gamma$ $7.00$ $0.08$ 1) $9.80$ $0.06$ 2) $8.03$ $0.02$ 3) $6.76$ $0.02$ 4) $4.20$ $0.13$ 5) $5.05$ $0.02$ 6) $5.60$ $0.02$ 7) $5.77$ $0.02$ Edge average distance (nm) $4.65$	x)	8.52	0.02			
z)4.080.02 $\gamma$ )2.420.06 $\alpha$ 5.220.06 $\beta$ 6.480.06 $\gamma$ 7.000.081)9.800.062)8.030.023)6.760.024)4.200.135)5.050.026)5.600.027)5.770.02Edge average distance (nm)4.65	w)	8.40	0.02			
$\gamma$ )2.420.06 $\alpha$ 5.220.06 $\beta$ 6.480.06 $\gamma$ 7.000.081)9.800.062)8.030.023)6.760.024)4.200.135)5.050.026)5.600.027)5.770.02Edge average distance (nm)4.65	z)	4.08	0.02			
$\alpha$ 5.220.06 $\beta$ 6.480.06 $\gamma$ 7.000.081)9.800.062)8.030.023)6.760.024)4.200.135)5.050.026)5.600.027)5.770.02Edge average distance (nm)4.65	y)	2.42	0.06			
$\beta$ $6.48$ $0.06$ $\gamma$ $7.00$ $0.08$ $1$ $9.80$ $0.06$ $2$ $8.03$ $0.02$ $3$ $6.76$ $0.02$ $4$ $4.20$ $0.13$ $5$ $5.05$ $0.02$ $6$ $5.60$ $0.02$ $7$ $5.77$ $0.02$ Edge average distance (nm) $4.65$	α	5.22	0.06			
γ       7.00       0.08         1)       9.80       0.06         2)       8.03       0.02         3)       6.76       0.02         4)       4.20       0.13         5)       5.05       0.02         6)       5.60       0.02         7)       5.77       0.02         Edge average distance (nm)       4.65	β	6.48	0.06			
1)       9.80       0.06         2)       8.03       0.02         3)       6.76       0.02         4)       4.20       0.13         5)       5.05       0.02         6)       5.60       0.02         7)       5.77       0.02         Edge average distance (nm)       4.65       4.65	γ	7.00	0.08			
2)     8.03     0.02       3)     6.76     0.02       4)     4.20     0.13       5)     5.05     0.02       6)     5.60     0.02       7)     5.77     0.02       Edge average distance (nm)     4.65	1)	9.80	0.06			
3)       6.76       0.02         4)       4.20       0.13         5)       5.05       0.02         6)       5.60       0.02         7)       5.77       0.02         Edge average distance (nm)       4.65       4.65	2)	8.03	0.02			
4)     4.20     0.13       5)     5.05     0.02       6)     5.60     0.02       7)     5.77     0.02       Edge average distance (nm)     4.65	3)	6.76	0.02			
5)     5.05     0.02       6)     5.60     0.02       7)     5.77     0.02       Edge average distance (nm)     4.57       Global average distance (nm)     4.65	4)	4.20	0.13			
6)         5.60         0.02           7)         5.77         0.02           Edge average distance (nm)         4.57         0.02           Global average distance (nm)         4.65         0.02	5)	5.05	0.02			
7)     5.77     0.02       Edge average distance (nm)     4.57       Global average distance (nm)     4.65	6)	5.60	0.02			
Edge average     4.57       distance (nm)     Global average       4.65	7)	5.77	0.02			
Global average 4.65	Edge average distance (nm)	4.57				
	Global average distance (nm)	4.65				

 Table S8. Estimation of Pt NP-Cl distances for P-egg for all k and %Cl considered.

T-flat									
k=1			k=1.5			k=0.5			
1%Cl			1%Cl			1%Cl			
Pt NP fixed	Distance PtNP- Cl (nm)	Exposition proportion	Pt NP fixed	Distance PtNP-Cl (nm)	Exposition proportion	Pt NP fixed	Distance PtNP-Cl (nm)	Exposition proportion	
Surface Po	sitions	Propertien	Surface Pos	sitions	proportion	Surface Positions			
а	0.74	0.58	а	0.58	0.58	a)	2.25	0.58	
b	2.00	0.16	b	0.69	0.16	b)	3.76	0.08	
с	2.00	0.26	с	3.00	0.26	c)	2.25	0.13	
Surface average distance (nm)	1.27		Surface average distance (nm)	1.23		d)	1.00	0.08	
Edge Positi	ons		Edge Positi	ons		e)	3.63	0.13	
Ø	0.23	0.5	Ø	0.23	0.50	Surface average distance (nm)	2.45		
d	0.9	0.43	d	0.90	0.50	Edge Positi	ons		
е	2.00	0.07	Edge average distance (nm)	0.57		Ø	0.23	0.38	
Edge average distance (nm)	0.65		Global average distance	0.71		f)	2.25	0.25	
Global average distance	0.78					g)	1.00	0.11	
			0.15%Cl edge saturation			i)	3.63	0.13	
0.35%Cl ed	ge saturation		Pt NP fixed	Distance PtNP-Cl (nm)	Exposition proportion	j)	4.14	0.13	
Pt NP fixed	Distance PtNP- Cl (nm)	Exposition proportion	Surface Pos	sitions		Edge average distance (nm)	1.77		
Surface Po	sitions		а	6.75	0.58	Global average distance	1.92		
а	4.50	0.58	b	3.00	0.16				
b	2.00	0.16	с	3.00	0.26	1.4%Cl edg	e saturation		
С	2.00	0.26	Surface average distance (nm)	5.18		Pt NP fixed position	Distance PtNP-Cl (nm)	Exposition proportion	
Surface average distance (nm)	3.45		Edge Positi	ons		Surface Pos	sitions		
Edge Positi	ons		Ø	0.23	0.50	a)	2.25	0.58	
Ø	0.23	0.50	d	6.75	0.16	b)	1.00	0.16	
d	4.50	0.16	е	3.00	0.07	c)	1.00	0.26	
е	2.00	0.07	f	10.88	0.26	Surface average distance (nm)	1.73		
f	7.25	0.26	Edge average distance (nm)	4.30		Edge Positi	ons		
Edge average distance (nm)	2.91		Global average distance	4.50		Ø	0.23	0.50	
Global average distance	3.03					d)	2.25	0.16	
			0.52%Cl			e)	1.00	0.07	
0.5%Cl			Surface Pos	sitions		f)	3.63	0.26	
Pt NP fixed position	Distance PtNP- Cl (nm)	Exposition proportion	а	0.81	0.58	Edge average distance (nm)	1.51		

Surface Positions			b	3.00	0.16	Global average distance	1.56	
а	1.53	0.58	с	3.00	0.26		I	
b	2.00	0.16	Surface	1.73				
		0.00	distance (nm)					
C	2.00	0.26	Edge Positi	ons				
average distance (nm)	1.73		Ø	0.23	0.50			
Edge Positi	ons		d	0.90	0.43			
Ø	0.23	0.50	е	3.00	0.07			
d	0.90	0.43	Edge average distance (nm)	0.72				
е	2.00	0.07	Global average distance	0.94				
Edge average distance (nm)	0.65							
Global average distance	0.88							
0.1%Cl								
Pt NP fixed	Distance PtNP-	Exposition						
Surface Po	sitions	propertien						
a)	4.50	0.29						
h)	12.12	0.29						
b)	4.92	0.16						
c)	2.00	0.13						
g)	11.00	0.13						
Surface average distance (nm)	7.30							
Edge Positi	ons	I						
Ø	0.23	0.13						
d	7.25	0.16						
j	2.00	0.13						
е	2.00	0.07						
f	11.00	0.07						
i	6.02	0.16						
Ι	4.00	0.13						
k	13.00	0.13						
Edge average distance (nm)	5.65							
Global average distance	6.01							
1.4%Cl								
Pt NP fixed	Distance PtNP-	Exposition						
position Surface Por	CI (nm) sitions	proportion						
a	0.58	0.58						

b	2.00	0.16
С	2.00	0.26
Surface average distance (nm)	1.18	
Edge Positi	ions	
Ø	0.23	0.50
d	0.90	0.43
е	2.00	0.07
Edge average distance (nm)	0.65	
Global average distance	0.76	

 Table S9. Calculated chlorine surface loadings for each model platelet morphology, k and %Cl.

Cl/nm²												
	k=0.5			k=1			k=1.5					
%w/wCl	T-flat	P-egg	%w/wCl	T-flat	P-egg	%w/wCl	T-flat	P-egg				
1	0.40	0.39	0.1	0.08	0.08	0.15	0.18	0.18				
1.4	0.57	-	0.35	0.28	-	0.52	0.63	0.61				
4.5	-	1.83	0.5	0.40	0.39	1	1.21	1.18				
			1	0.81	-	1.21	1.47	1.43				
			1.2	-	0.94							
			1.4	1.14	1.10							

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