Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Al-Pt compounds catalyzing the oxygen evolution reaction

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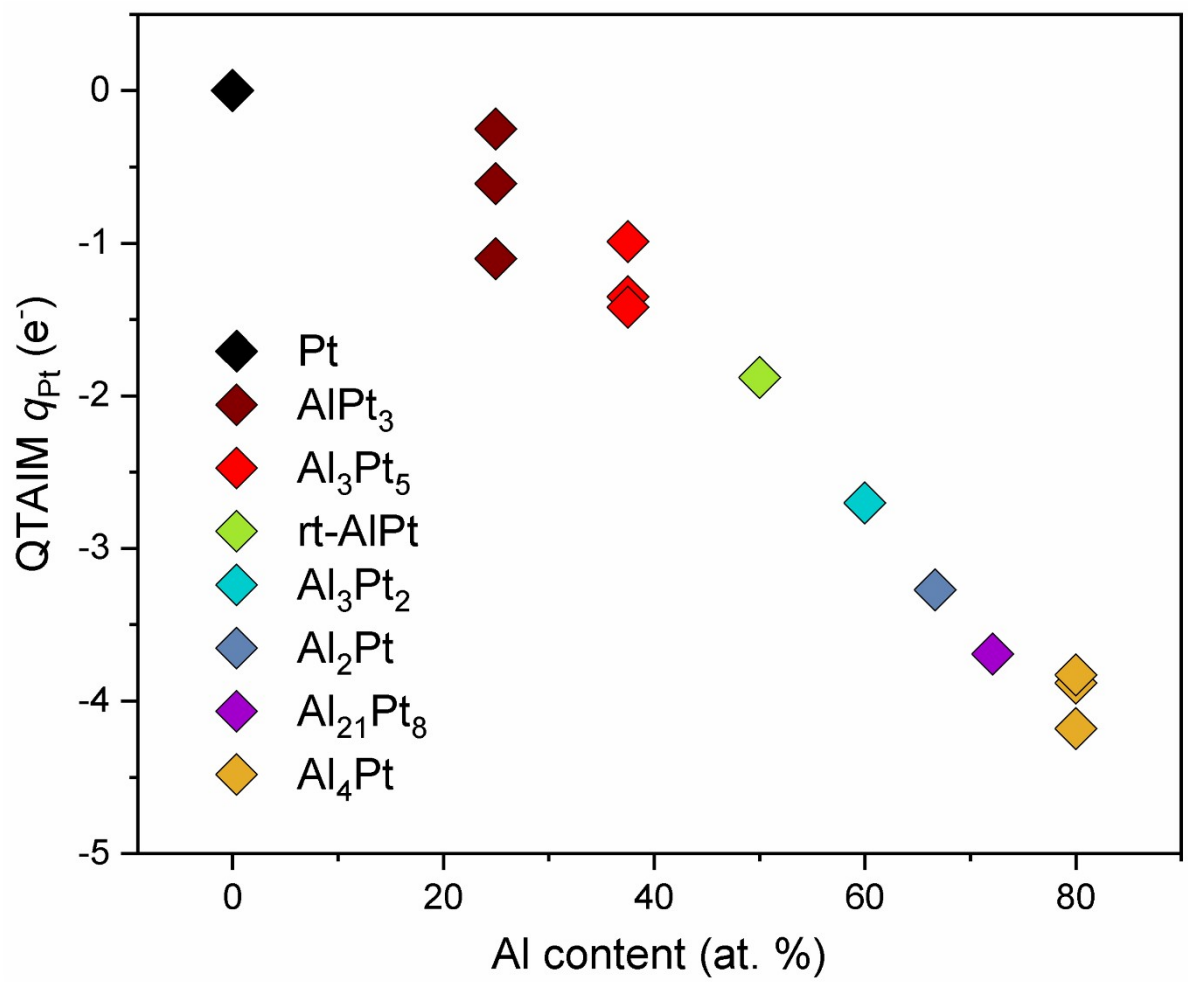

Figure S1. QTAIM charges of Pt atoms as function of Al content in different Al-Pt compounds. The values are taken from [1], with exception of those for rt-AlPt (calculated in this work). The multiple points of same colour represent the different Pt atoms in the crystal structure.

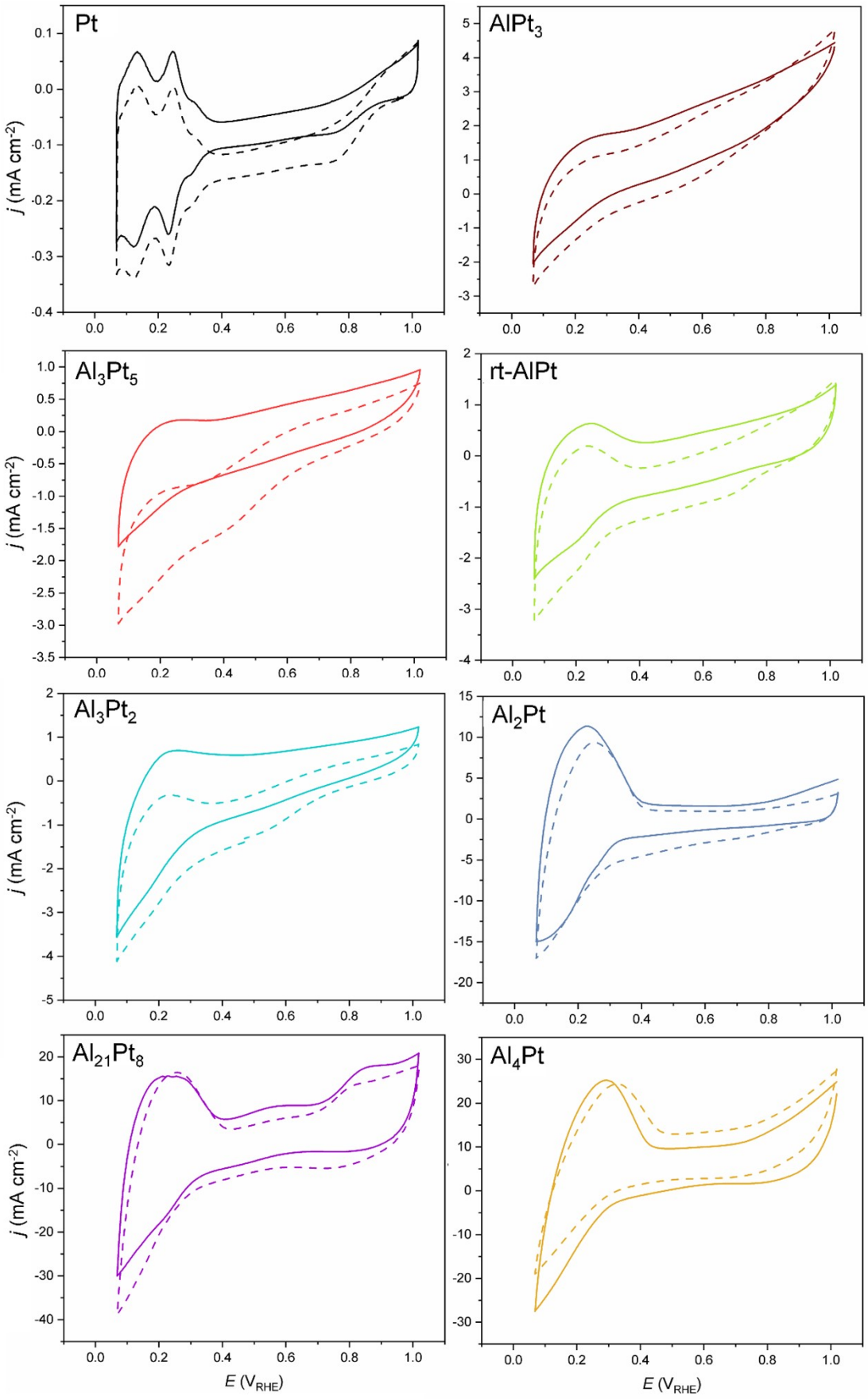

Figure S2. Cyclic voltammograms for the Al-Pt compounds and elemental Pt: 6th (*dashed*) and 50th (*solid*) cycles are shown.

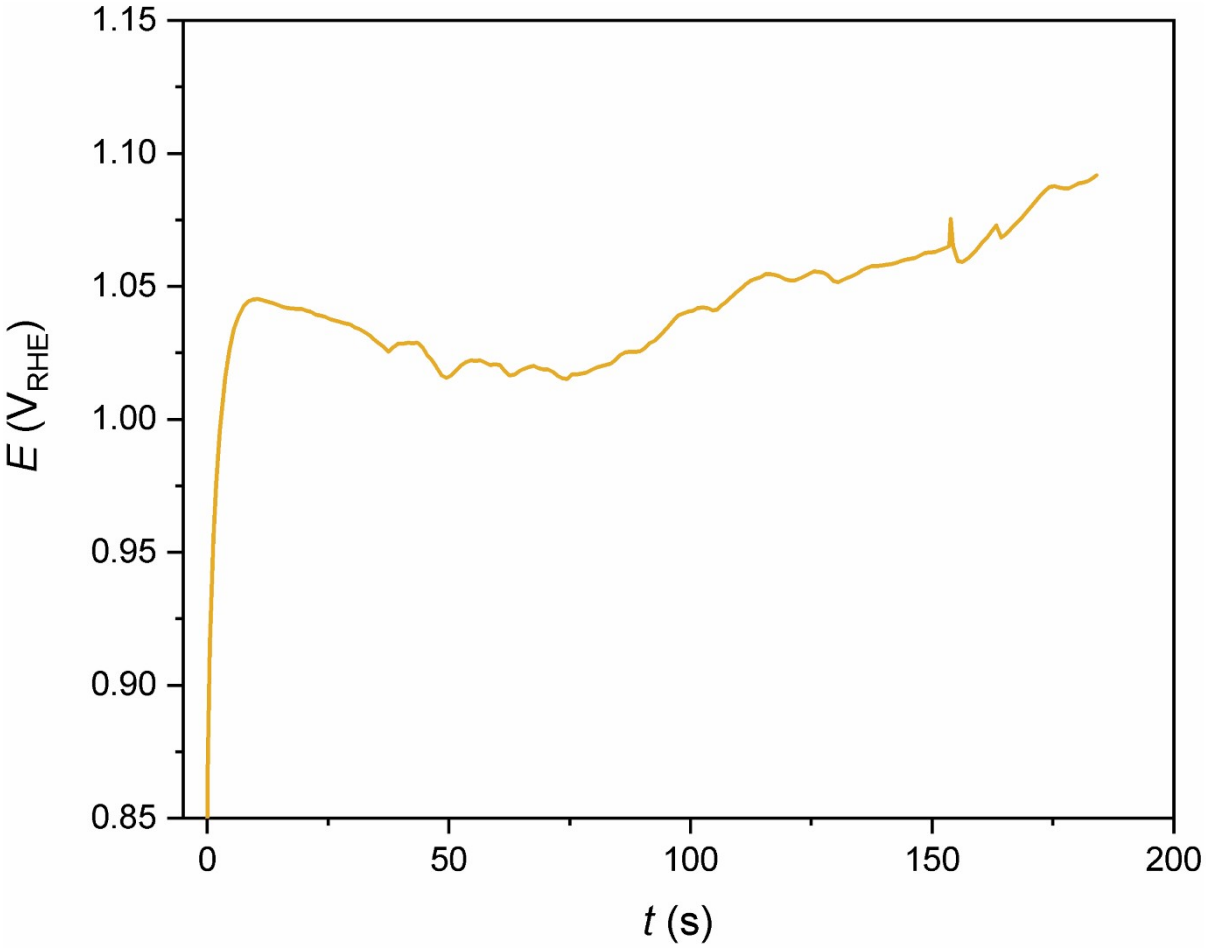

Figure S3. Chronopotentiometry for Al_4Pt at current density of 10 mA cm^{-2}.

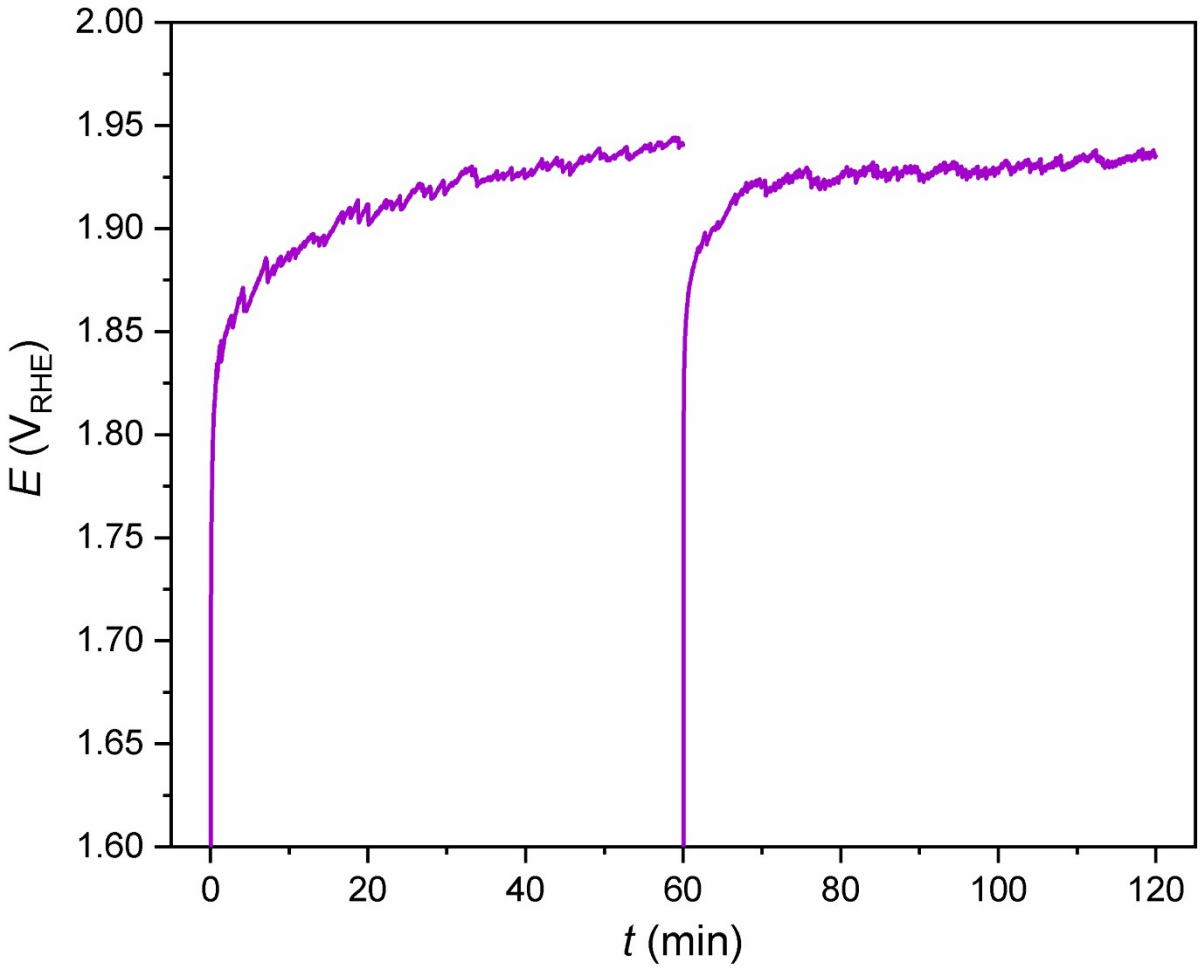

Figure S4. Chronopotentiometry for $Al_{21}Pt_8$ at current density of 10 mA cm^{-2}.

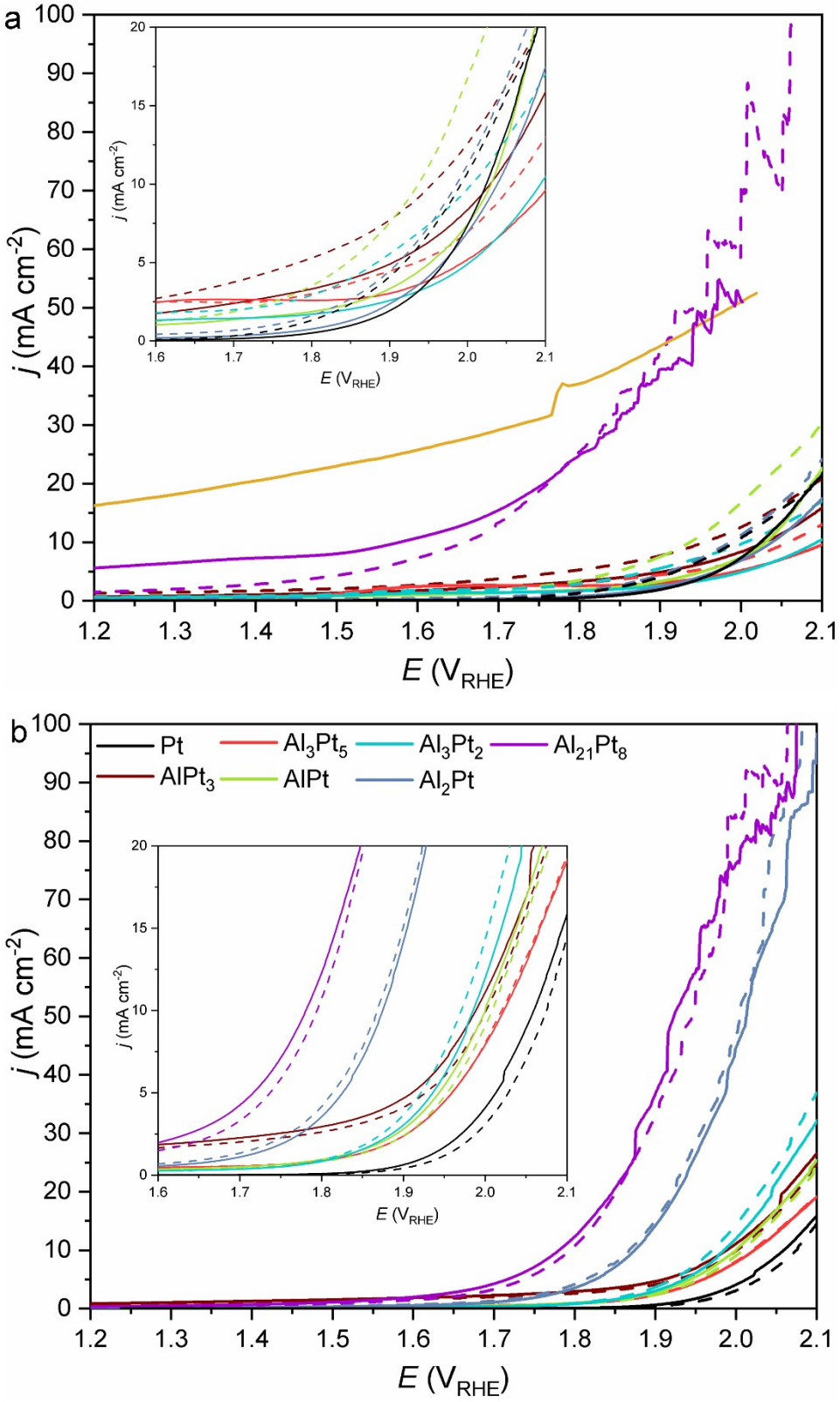

Figure S5. Linear sweep voltammograms with the Al-Pt compounds as anode materials: a) initial (*solid lines*) and after the cyclic voltammetry (*dashed lines*), and b) after one (*solid lines*) and two hours (*dashed lines*) of chronopotentiometry at the current density of 10 mA cm^{-2}. Insets: enlargement of linear sweep voltammograms in the region from 0 to 20 mA cm^{-2}. The *orange* curve (a) represents initial LSV with Al_4Pt electrode.

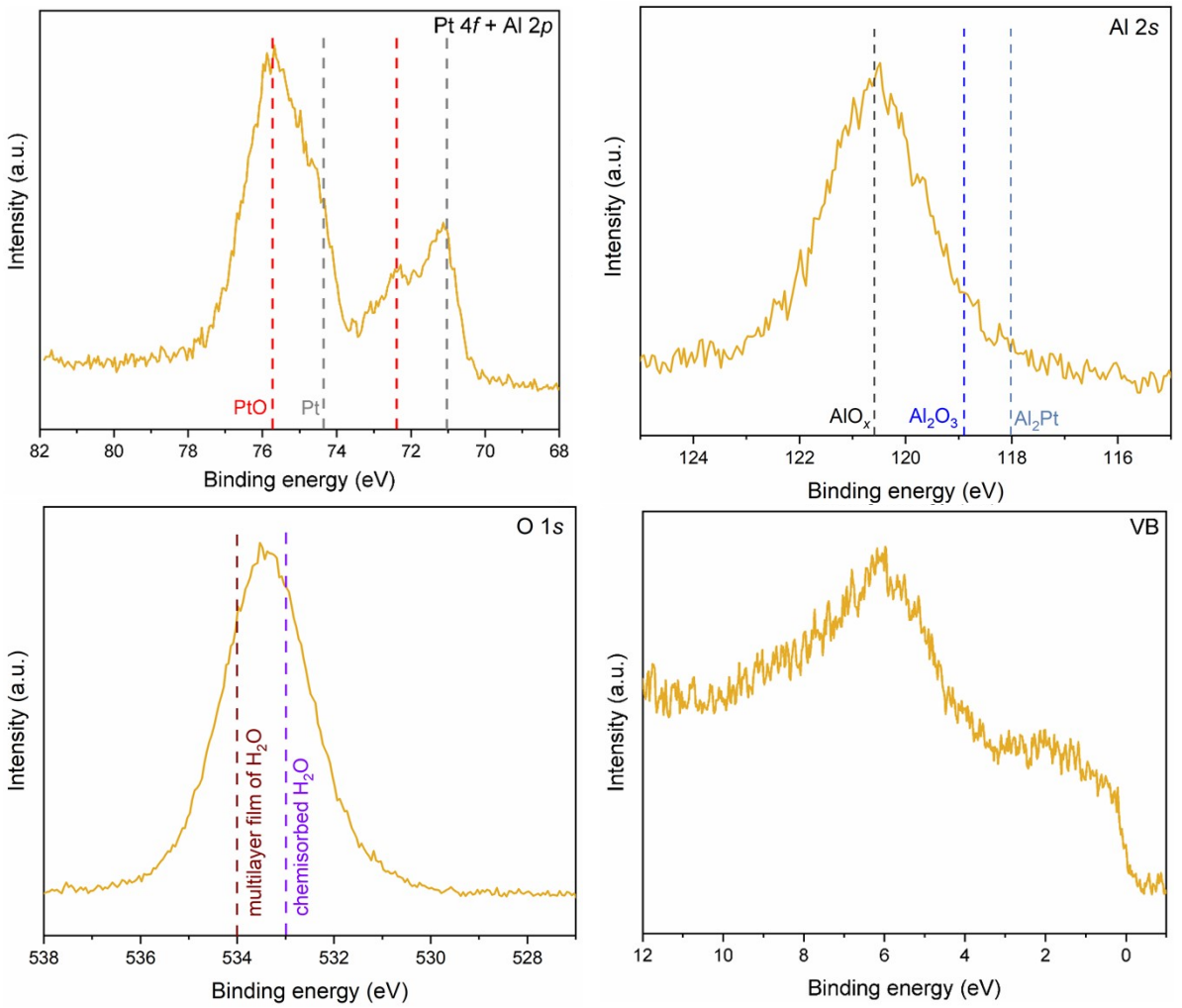

Figure S6. XPS spectra of the Pt 4*f*, Al 2*s*, O 1*s* core levels and valence band for the Al_4Pt compound after 200 s of chronopotentiometry at current density of 10 mA cm^{-2}.

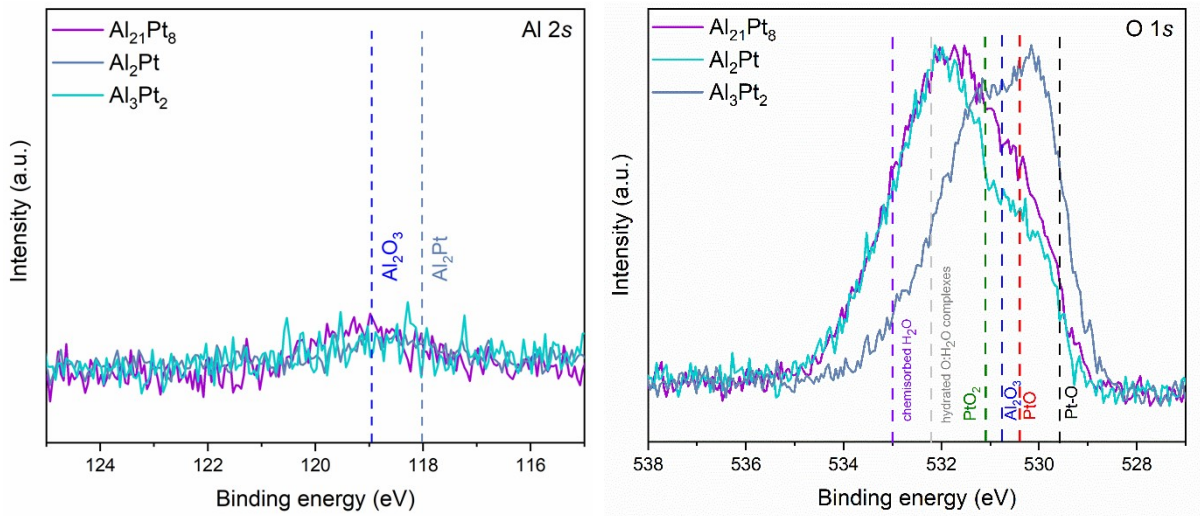

Figure S7. Normalized XPS spectra of the Al 2*s* and O 1*s* core levels for the selected Al-Pt compounds after 2 h of chronopotentiometry at current density of 10 mA cm^{-2}.

Table S1. Experimental details on homogenization annealing of Al-Pt compounds.

Compound	*T*, °C	*t*, days
rt-$AlPt_3$	1000	35
Al_3Pt_5	1000	35
rt-AlPt	1000	21
Al_3Pt_2	1000	21
Al_2Pt	1000	26
$Al_{21}Pt_8$	600	28
	1000	14
Al_4Pt	600	28
	780	14

Table S2. SPS densification of the Al-Pt samples.

Compound	SPS conditions		
	T_{max}, °C	*t*, min	*P*, MPa
Pt	1200	10	80
rt-$AlPt_3$	1000	10	80
Al_3Pt_5	1000	3	80
rt-AlPt	1000	3	80
Al_3Pt_2	1000	5	80
Al_2Pt	1000	10	80
$Al_{21}Pt_8$	900	10	80
Al_4Pt	700	-	80

Table S3. Lattice parameters of the Al-Pt intermetallic compounds.

Compound	Structure type	Space group	Lattice parameters, Å		
			a	***b***	***c***
rt-$AlPt_3$	$GaPt_3$	*P*4/*mbm*	5.4655(3)	*a*	7.8005(7)
Al_3Pt_5	Ge_3Rh_5	*Pbam*	5.4143(6)	10.732(1)	3.9636(5)
rt-AlPt	FeSi	$P2_13$	4.8656(1)	*a*	*a*
Al_3Pt_2	Ni_2Al_3	$P\bar{3}m1$	4.2050(2)	*a*	5.1721(2)
Al_2Pt	*anti*-CaF_2	$Fm\bar{3}m$	5.9243(2)	*a*	*a*
$Al_{21}Pt_8$	$Al_{21}Pt_8$	$I4_1/a$	12.9531(2)	*a*	10.6667(3)
Al_4Pt	Al_4Pt	*P*3*c*1	13.0769(2)	*a*	9.6367(3)

Table S4. The concentrations of Al in the electrolyte (C, mg L^{-1}) after 2h CP experiments with various Al-Pt compounds

Compound	***C*(Al), mg L^{-1}**
rt-$AlPt_3$	< 0.001
Al_3Pt_5	0.9
rt-AlPt	0.12
Al_3Pt_2	< 0.001
Al_2Pt	0.23
$Al_{21}Pt_8$	3.32
Al_4Pt	11.39

Table S5. Pt 4*f* core levels positions for the Al-Pt intermetallic compounds.*

Compound	**Binding energy, eV**	
	Pt $4f_{5/2}$	Pt $4f_{7/2}$
Pt	74.2	70.9
rt-$AlPt_3$	74.5	71.2
Al_3Pt_5	75.3	72.0
rt-AlPt	75.2	71.9
Al_3Pt_2	75.6	72.3
Al_2Pt	75.6	72.3
$Al_{21}Pt_8$	76.1	72.8
Al_4Pt	76.1	72.8

*Taken from HAXPES data [2] and estimated at maximum peak intensity.

References:

[1] Baranov, A., Kohout, M., Wagner, F.R., Grin, Y., Bronger, W. // *Z. Kristallogr.* **2007**, *222*, 527-531.

[2] I. Antonyshyn, O. Sichevych, U. Burkhardt, A.M. Barrios Jiménez, D. Takegami, A. Melendez-Sans, Y.-F. Liao, K.-D. Tsuei, D. Kasinanthan and A. Ormeci, *submitted*.