

Electronic Supplementary Information

Impregnation of KOAc on PdAu/SiO₂ causes Pd-acetate formation and metal restructuring

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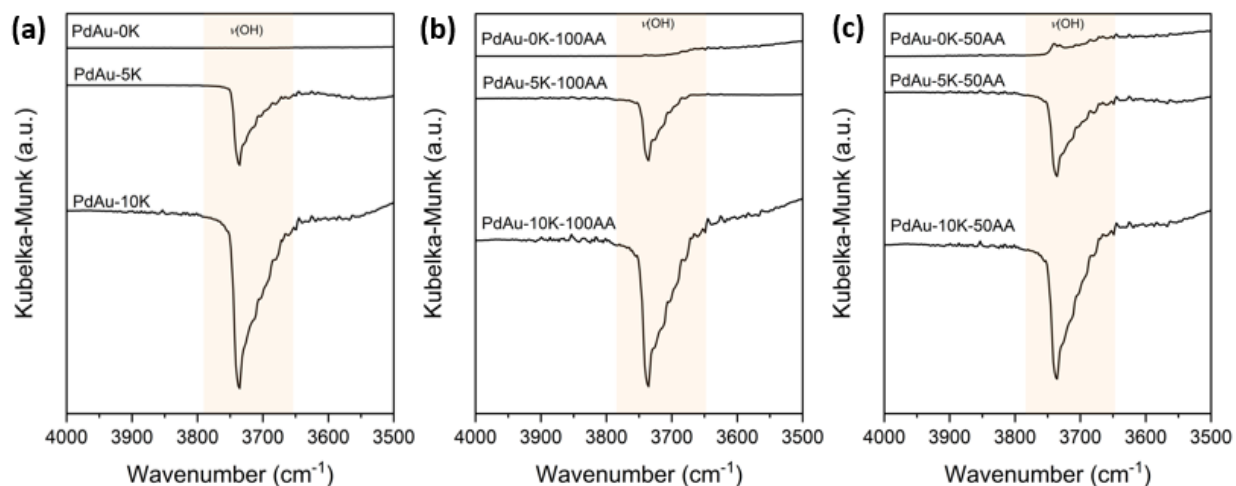


Figure S1. DRIFTS spectra in the 4000 – 3500 cm⁻¹ ν(OH) region of the PdAu/SiO₂ containing 0, 5, and 10 wt% K treated in (a) 0, (b) 100, and (c) 50 vol% AcOH solutions showing negative ν(OH) peaks associated with conversion of isolated silanols to either silyl acetates or alkali silanolates. As-synthesized PdAu/SiO₂ was used as background for all samples.

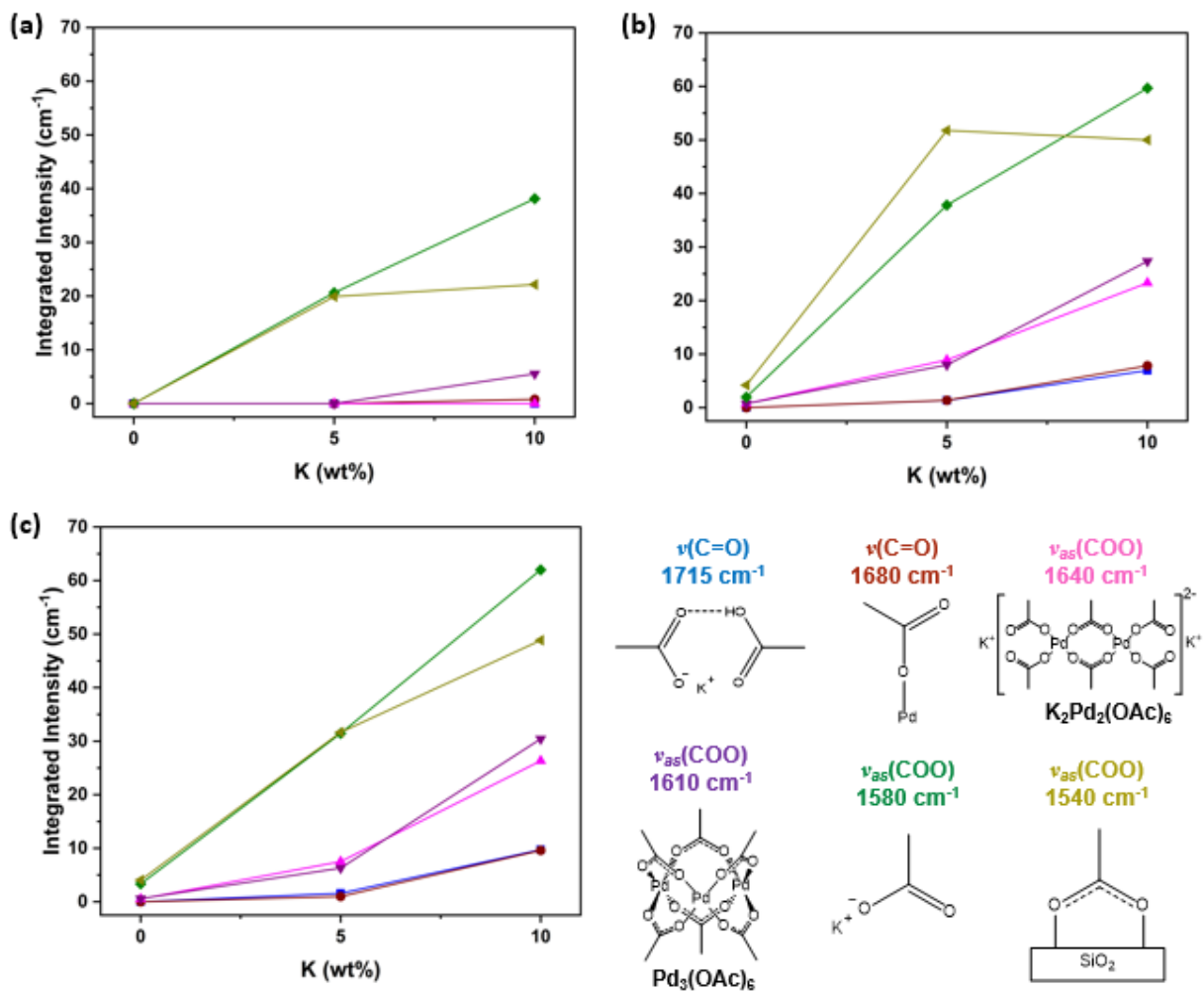


Figure S2. Integrated intensities of $\nu(\text{C}=\text{O})$ and $\nu_{\text{as}}(\text{COO})$ peaks associated with various Pd-acetates determined by deconvoluted DRIFTS spectra of the PdAu/SiO₂ treated in (a) 0, (b) 100, and (c) 50 vol% AcOH solutions versus K wt% loading.

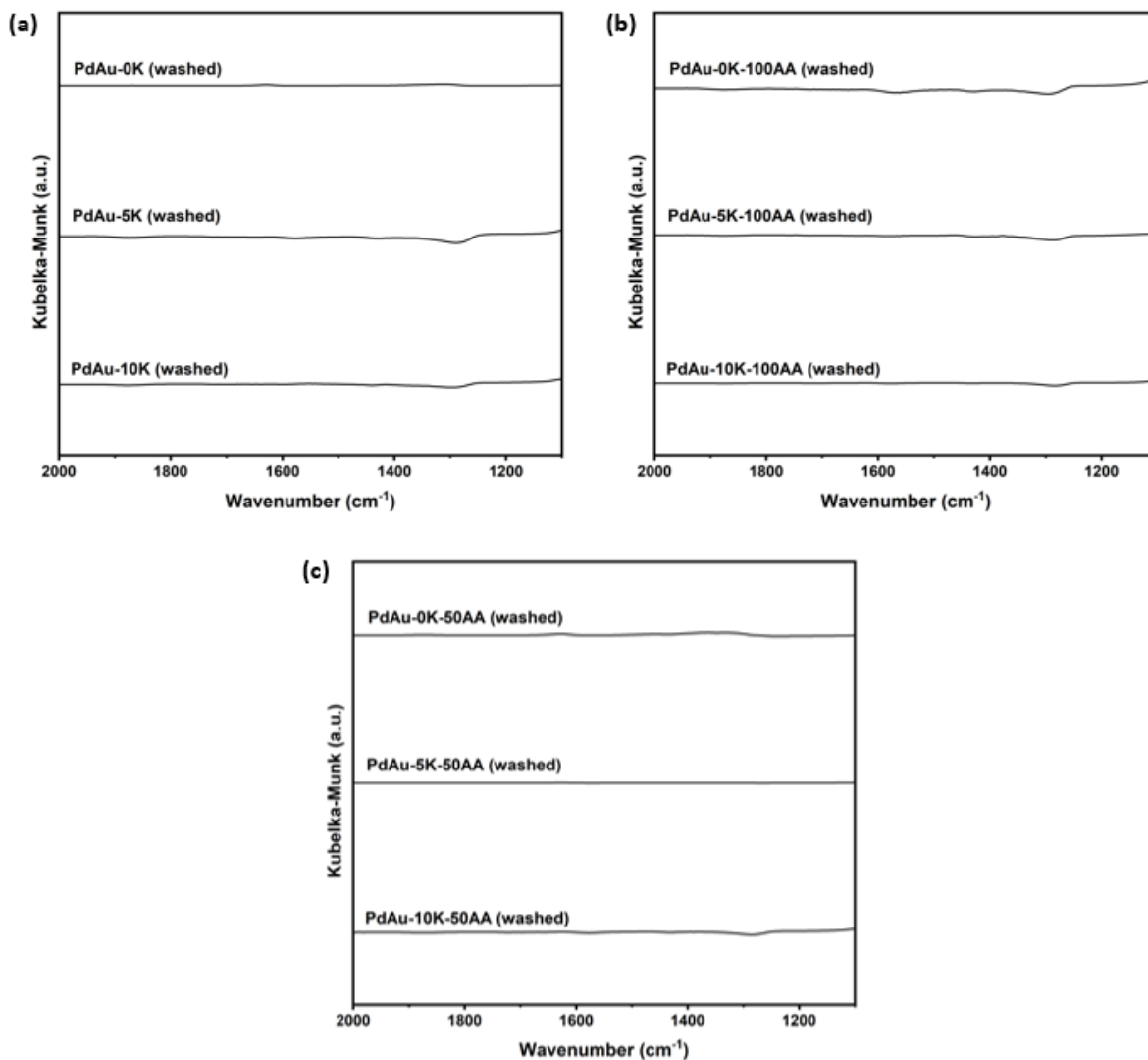


Figure S3. DRIFTS spectra in the 2000 – 1100 cm^{-1} acetate region of the PdAu/SiO₂ containing 0, 5, and 10 wt% K treated in (a) 0, (b) 100, and (c) 50 vol% AcOH solutions after washing with water and drying overnight showing disappearance of acetate vibrational modes. As-synthesized PdAu/SiO₂ was used as background for all samples.

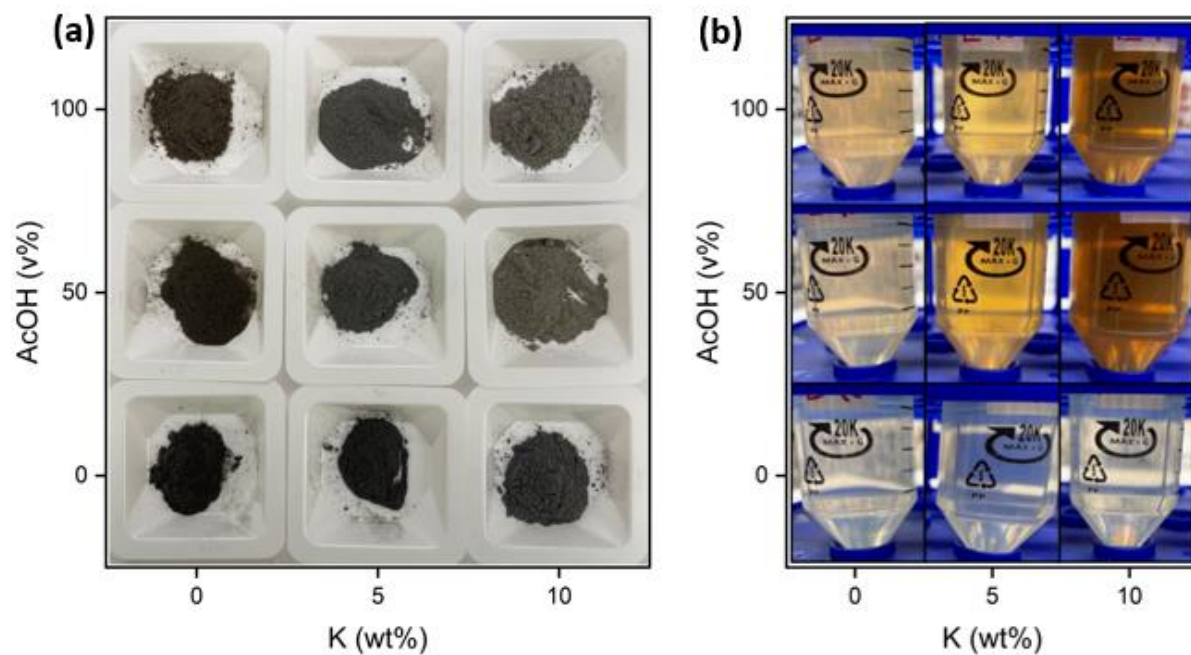


Figure S4. (a) PdAu/SiO₂ samples after wet impregnation and (b) filtrate collected after washing PdAu/SiO₂ samples with water showing color change versus AcOH vol% and K wt% loading.

Table S1. XANES energy and EXAFS fitting results for samples at Au L_{III} edge

Sample	XANES Energy (keV)	Scattering path	CN ($\pm 10\%$)	R (\AA) ($\pm 0.02 \text{\AA}$)	$\Delta\sigma^2$ ($\times 10^3 \text{\AA}$)	E_0 (eV)
Au foil	11.9190	Au-Au	12	2.87	0.0	3.9
PdAu/SiO ₂	11.9181	Au-Au	5.1	2.82	0.0	2.4
		Au-Pd	6.4	2.77	0.0	2.7
PdAu-0K ^a	11.9180	Au-Au	-	-	-	-
		Au-Pd	-	-	-	-
PdAu-5K	11.9182	Au-Au	5.1	2.79	0.0	-2.3
		Au-Pd	6.3	2.76	0.0	3.9
PdAu-10K	11.9183	Au-Au	4.9	2.79	0.0	-1.8
		Au-Pd	6.4	2.76	0.0	3.9
PdAu-0K-50AA	11.9182	Au-Au	4.5	2.79	0.0	-1.9
		Au-Pd	6.6	2.77	0.0	5.6
PdAu-5K-50AA (a) ^a	11.9182	Au-Au	-	-	-	-
		Au-Pd	-	-	-	-
PdAu-5K-50AA (b) ^a	11.9182	Au-Au	-	-	-	-
		Au-Pd	-	-	-	-
PdAu-5K-50AA (c)	11.9184	Au-Au	4.3	2.82	0.0	-0.6
		Au-Pd	6.0	2.77	0.0	4.6
PdAu-10K-50AA ^a	11.9182	Au-Au	-	-	-	-
		Au-Pd	-	-	-	-
PdAu-0K-100AA	11.9181	Au-Au	4.6	2.80	0.0	-2.5
		Au-Pd	6.5	2.77	0.0	4.7
PdAu-5K-100AA	11.9184	Au-Au	5.3	2.80	0.0	-2.9
		Au-Pd	6.3	2.76	0.0	4.1
PdAu-10K-100AA	11.9185	Au-Au	5.7	2.82	0.0	0.5
		Au-Pd	5.7	2.77	0.0	3.9

^aData was too noisy for reliable EXAFS fitting.

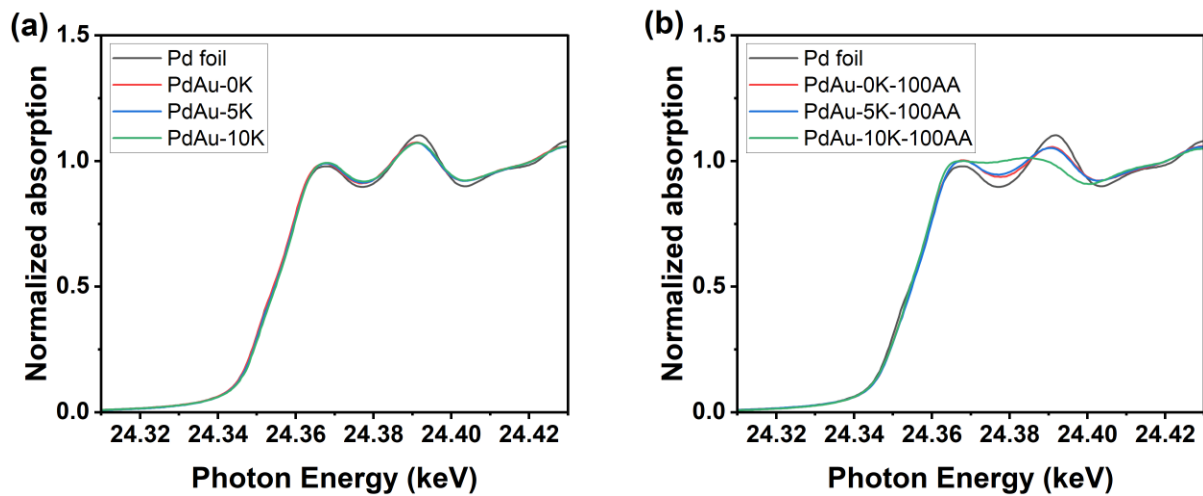


Figure S5. Pd K edge XANES for the Pd foil (black) and KOAc-impregnated PdAu/SiO₂ samples containing 0 (red), 5 (blue), and 10 (green) wt% K treated in either (a) water or (b) AcOH solution.

Table S2. XANES energy and EXAFS fitting results for samples at Pd K edge

Sample	XANES Energy (keV)	Scattering path	CN ($\pm 10\%$)	R (\AA) ($\pm 0.02 \text{\AA}$)	$\Delta\sigma^2$ ($\times 10^3 \text{\AA}$)	E_0 (eV)
Pd foil	24.3503	Pd-Pd	12	2.75	-	-
PdAu/SiO ₂	24.3508	Pd-Pd	7.7	2.74	1.0	2.7
		Pd-Au	2.4	2.74	1.0	-1.9
PdAu-0K	24.3498	Pd-Pd	7.6	2.75	1.0	3.3
		Pd-Au	2.3	2.75	1.0	-1.5
PdAu-5K	24.3506	Pd-Pd	7.3	2.74	1.0	2.6
		Pd-Au	2.6	2.74	1.0	-0.9
PdAu-10K	24.3511	Pd-Pd	7.4	2.75	1.0	3.1
		Pd-Au	2.6	2.75	1.0	-1.2
PdAu-0K-50AA	24.3502	Pd-Pd	7.1	2.75	1.0	2.3
		Pd-Au	2.4	2.75	1.0	-2.0
PdAu-5K-50AA (a)	24.3519	Pd-O	1.0	2.02	0.0	-3.6
		Pd-Pd	6.0	2.75	1.0	-6.4
		Pd-Au	1.4	2.75	1.0	-7.5
PdAu-5K-50AA (b)	24.3511	Pd-O	1.3	2.02	0.0	6.5
		Pd-Pd	5.6	2.75	1.0	2.1
		Pd-Au	1.3	2.75	1.0	-1.0
PdAu-5K-50AA (c)	24.3529	Pd-O	1.3	2.02	0.0	6.2
		Pd-Pd	5.3	2.75	1.0	2.6
		Pd-Au	1.2	2.75	1.0	3.1
PdAu-10K-50AA	24.3537	Pd-O	2.5	2.02	0.0	2.1
		Pd-Pd	3.5	2.75	1.0	-1.5
		Pd-Au	0.5	2.75	1.0	3.8
PdAu-0K-100AA	24.3514	Pd-O	0.9	2.02	0.0	5.9
		Pd-Pd	6.4	2.75	1.0	2.9
		Pd-Au	1.8	2.75	1.0	0.0
PdAu-5K-100AA	24.3509	Pd-O	1.0	2.02	0.0	6.1
		Pd-Pd	6.2	2.75	1.0	1.9
		Pd-Au	1.4	2.75	1.0	-1.0
PdAu-10K-100AA	24.3535	Pd-O	2.3	2.02	0.0	2.9
		Pd-Pd	3.9	2.75	1.0	-1.1
		Pd-Au	0.6	2.75	1.0	3.1

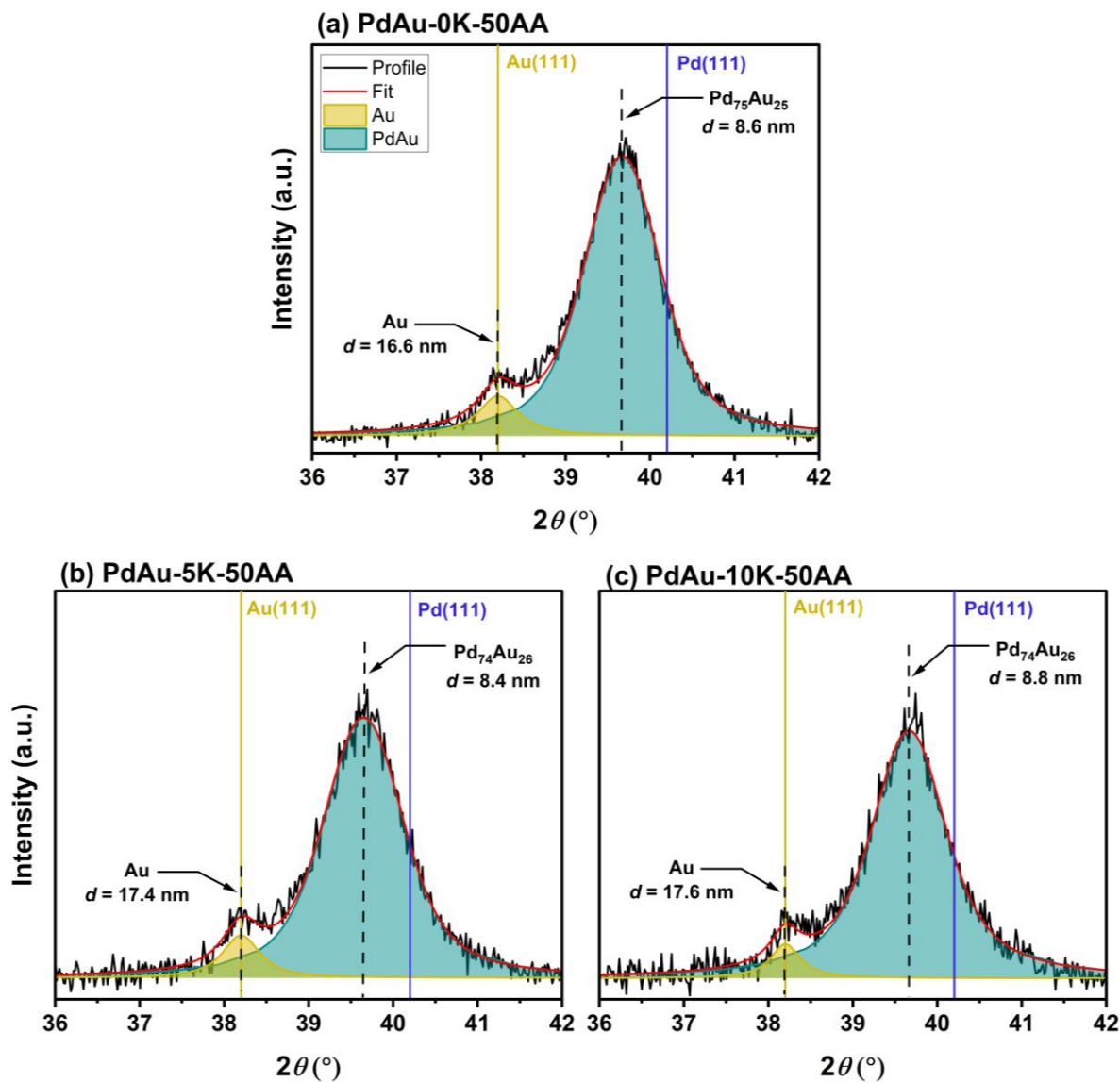


Figure S6. XRD profiles of the (a) PdAu/SiO₂ treated in 50 vol% AcOH (PdAu-0K-50AA) and KOAc-impregnated PdAu/SiO₂ treated in 50 vol% AcOH containing (b) 5 wt% K (PdAu-5K-50AA) and (c) 10 wt% K (PdAu-10K-50AA). Blue line represents Pd(111) reference, and the gold line represents Au(111) reference. Green curve represents the Pd-rich PdAu alloy phase, and the gold curve represents pure Au phase.

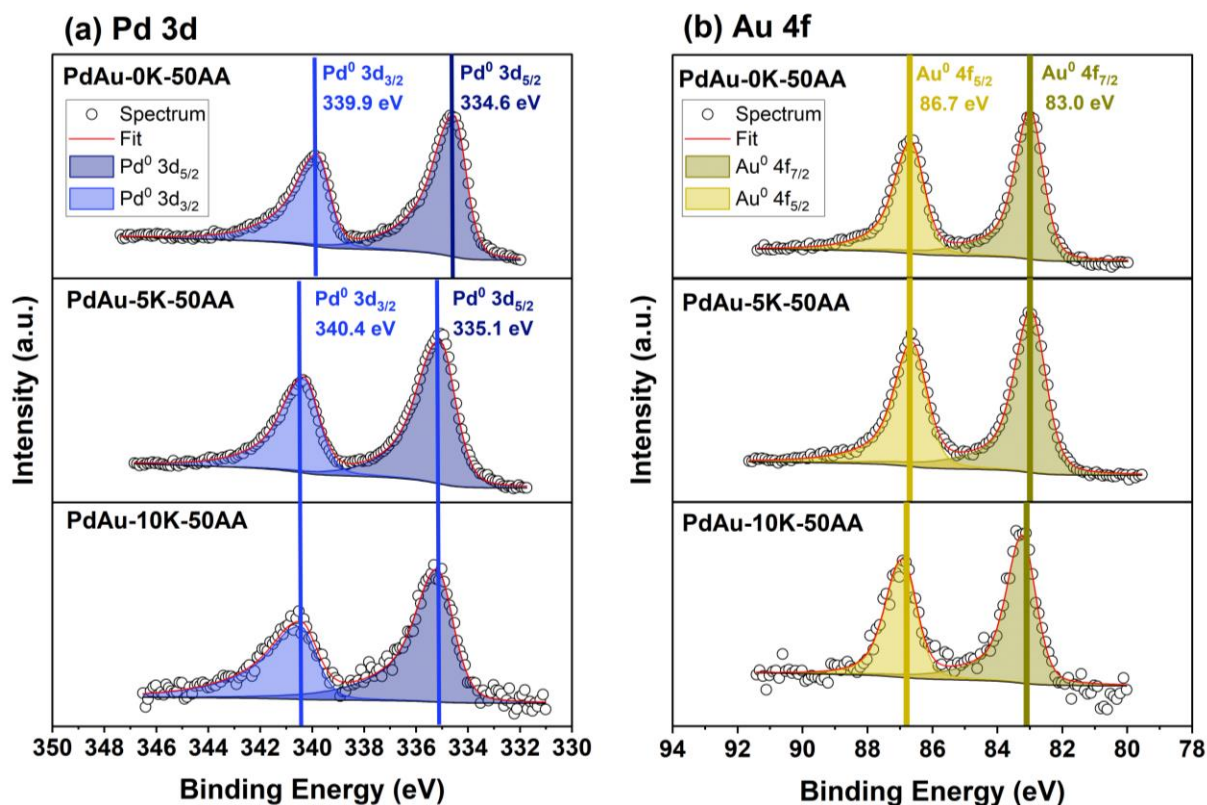


Figure S7. XPS spectra at the (a) Pd 3d and (b) Au 4f core levels of the PdAu/SiO₂ treated in 50 vol% AcOH (PdAu-0K-50AA) and KOAc-impregnated PdAu/SiO₂ treated in 50 vol% AcOH containing 5 wt% K (PdAu-5K-50AA) and 10 wt% K (PdAu-10K-50AA). BE values are ± 0.1 eV.

Table S3. Phase compositions, grain sizes, and Pd:Au surface ratio of 50 vol% AcOH/KOAc-treated PdAu/SiO₂.

Sample	Phase composition ^a (at%)	Grain size ^b (nm)	Pd:Au surface ratio ^c (at%)
PdAu-0K-50AA	Au	16.4	77:23
	Pd ₇₅ Au ₂₅	8.6	
PdAu-5K-50AA (a)	Au	15.6	73:27
	Pd ₇₄ Au ₂₆	8.4	
PdAu-5K-50AA (b)	Au	19.0	74:26
	Pd ₇₆ Au ₂₄	8.6	
PdAu-5K-50AA (c)	Au	17.4	74:26
	Pd ₇₆ Au ₂₄	8.3	
PdAu-10K-50AA	Au	17.6	73:27
	Pd ₇₆ Au ₂₄	8.8	

^aCalculated from XRD data using Vegard's equation.

^bCalculated from XRD data using Scherrer's equation.

^cCalculated from XPS data at Pd 3d and Au 4f core levels.

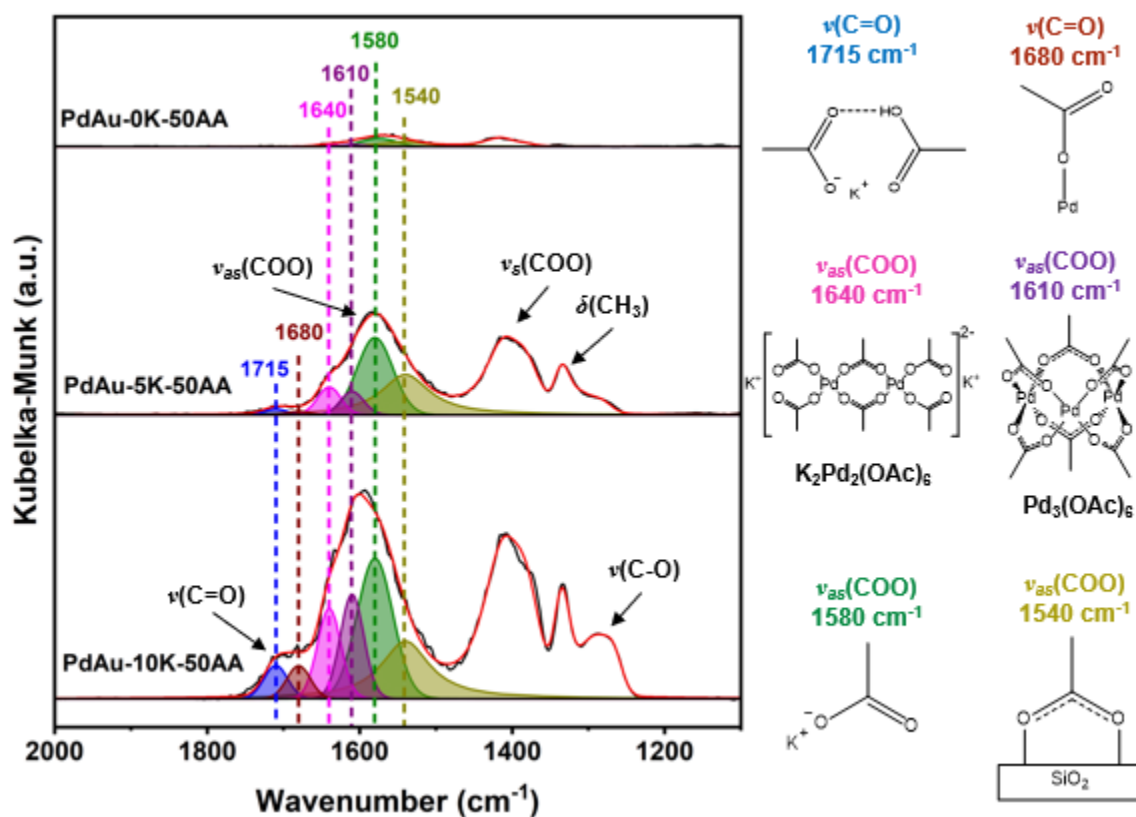


Figure S8. Deconvoluted DRIFTS spectra in the 2000 – 1100 cm^{-1} acetate region of the PdAu/SiO₂ treated in 50 vol% AcOH (PdAu-0K-50AA) and KOAc-impregnated PdAu/SiO₂ treated in 50 vol% AcOH containing 5 wt% K (PdAu-5K-50AA) and 10 wt% K (PdAu-10K-50AA). $\nu(\text{C}=\text{O})$ peaks are located between 1800 – 1670 cm^{-1} . $\nu_{\text{as}}(\text{COO})$ peaks are located between 1670 – 1500 cm^{-1} . $\nu_{\text{s}}(\text{COO})$ peaks are located between 1450 – 1390 cm^{-1} . $\delta(\text{CH}_3)$ peaks are located between 1390 – 1300 cm^{-1} . $\nu(\text{C}-\text{O})$ peaks are located between 1300 – 1250 cm^{-1} . As-synthesized PdAu/SiO₂ was used as background for all samples.

Table S4. ICP-OES analysis of metals recovered in filtrate after washing 50 vol% AcOH/KOAc-treated samples with water.

Sample	Pd recovered (% of initial)	Au recovered (% of initial)	K recovered (% of initial)
PdAu-0K-50AA	4.6	0	-
PdAu-5K-50AA (a)	15.9	0	99
PdAu-5K-50AA (b)	16.0	0	95
PdAu-5K-50AA (c)	15.9	0	90
PdAu-10K-50AA	32.3	0	95

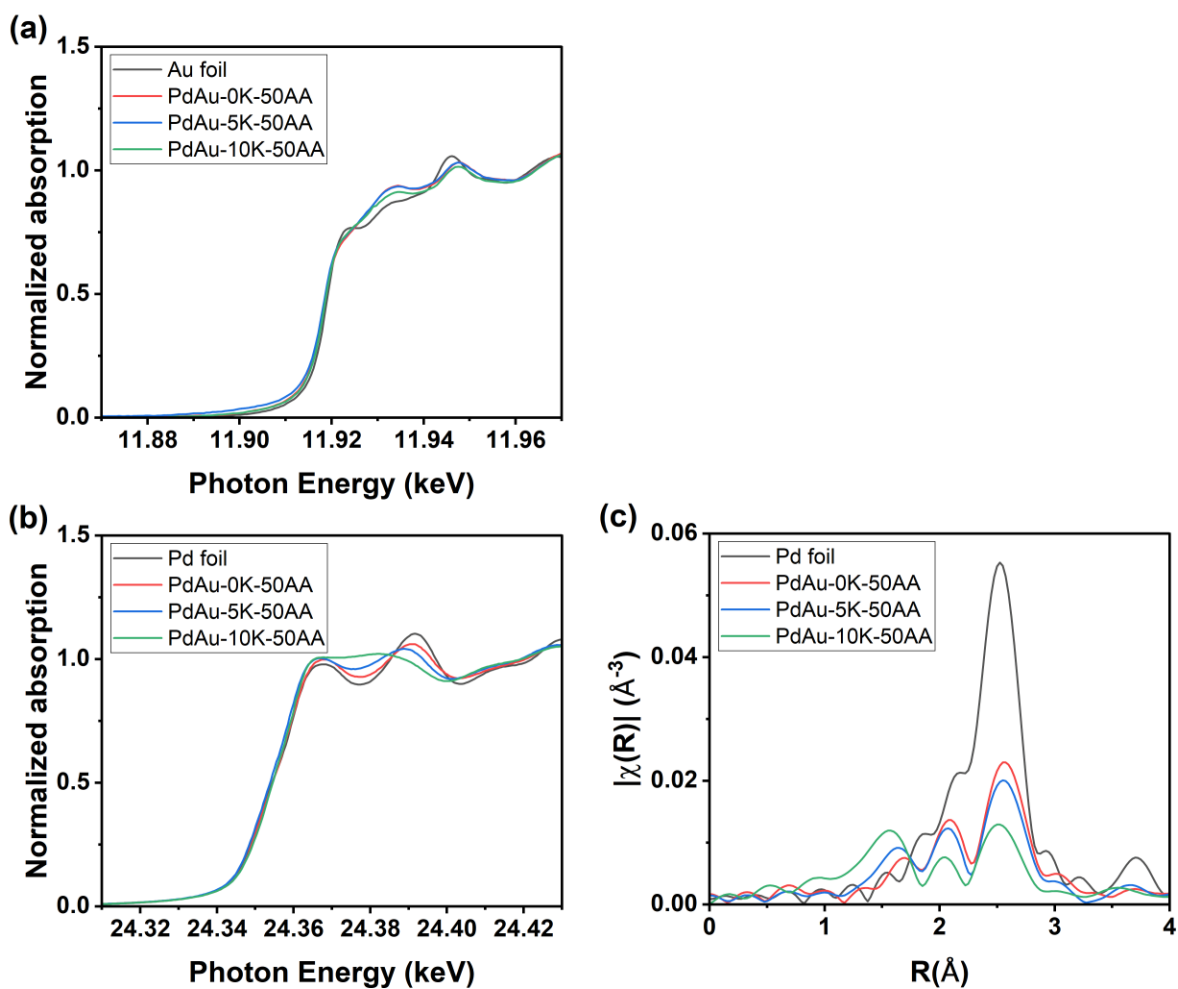


Figure S9. (a) Au L_{III} edge XANES, (b) Pd K edge XANES, and (c) Pd K edge EXAFS for the Pd foil (black) and KOAc-impregnated PdAu/SiO₂ samples containing 0 (red), 5 (blue), and 10 (green) wt% K treated in 50 vol% AcOH (v/v in water) solution.

Design of Experiments (DOE) and Statistical Analysis

Statistical analysis based on the design of experiments (DOE) presented in Table 1 of the Main Text was performed on 8 response variables selected from XRD, XPS, DRIFTS, XAS, and ICP-OES data: 1) Au grain size, 2) PdAu grain size, 3) Pd surface content, 4) Pd²⁺ content, 5) monodentate acetate content on surface Pd, 6) Pd₃(OAc)₆ content, 7) K₂Pd₂(OAc)₆ content, and 8) Pd loss after washing. The values of the responses are summarized in Tables S5 – S7 based on the AcOH vol% and K wt% treatments for each sample.

Each of the responses were fit using Minitab software based on a least-squares linear regression model containing all linear, quadratic, and interaction effects of the two factors AcOH vol% and K wt% (Equation 3 in the Main Text). The response surface plots are presented in Figures 9 and 10 of the Main Text. The fitting coefficients and their standard errors for all the response surface plots are presented in Tables S8 – S15.

Coded coefficients were also calculated in Minitab by centering and scaling the variables so that the low and high factor levels coded as -1 and 1, respectively. The transformation to coded coefficients is necessary in order to orthogonalize the factors and isolate the factor effects, allowing for relative comparisons between different effects. For example, a larger coded coefficient means that effect has a greater relative contribution to the response surface model. The coded coefficients and their standard errors for each response are also presented in Tables S8 – S15.

The coded coefficients are then used to analyze which effects have statistically significant contributions to the response surface models. The *t*-values for each coefficient are calculated as the ratio between the value of the coefficient and its standard error. The two-tailed *p*-values are then calculated by the following equation:

$$p = 2 * (1 - P(T \leq |t|, d.f.)) \quad (S1)$$

where $|t|$ is the absolute value of the *t*-value, *d.f.* is the degree of freedom calculated by subtracting the number of coefficients from total number of runs (*d.f.* = 5 for a model with 6 coefficients and 11 runs), and $P(T \leq |t|, d.f.)$ is the cumulative distribution function for a *t*-distribution at a particular *t*-value and degree of freedom. The calculated *t*-values and *p*-values are included in Tables S8 – S15. At the 95% confidence level ($\alpha = 0.05$) with 5 degrees of freedom, $p \leq 0.05$ and $t \geq 2.571$ indicate statistical significance. Plotting the absolute value of the *t*-values in a Pareto chart of the standardized effects offers a visual representation to determine the degree of statistical significance for each factor (Figures S9 – S16).

Table S5. Au and Pd_xAu_y grain size responses from experimental design.

Run	Sample	AcOH (vol%)	K (wt%)	Grain Size (nm)	
				Au	Pd _x Au _y
1	PdAu-0K	0	0	13.4	8.3
2	PdAu-5K	0	5	13.4	8.1
3	PdAu-10K	0	10	14.4	8.1
4	PdAu-0K-50AA	50	0	16.4	8.6
5	PdAu-5K-50AA (a)	50	5	15.6	8.4
6	PdAu-5K-50AA (b)	50	5	19.0	8.6
7	PdAu-5K-50AA (c)	50	5	17.4	8.3
8	PdAu-10K-50AA	50	10	17.6	8.8
9	PdAu-0K-100AA	100	0	20.2	8.6
10	PdAu-5K-100AA	100	5	18.1	8.3
11	PdAu-10K-100AA	100	10	14.9	8.4

Table S6. Pd surface content, Pd²⁺ content, and Pd loss responses from experimental design.

Run	Sample	AcOH (vol%)	K (wt%)	Pd surface content (at%)	Pd ²⁺ content (% of Pd)	Pd loss (%)
1	PdAu-0K	0	0	80	0	0.7
2	PdAu-5K	0	5	79	0	1.7
3	PdAu-10K	0	10	77	0	2.1
4	PdAu-0K-50AA	50	0	77	0	4.5
5	PdAu-5K-50AA (a)	50	5	73	25	15.9
6	PdAu-5K-50AA (b)	50	5	74	32.5	16.0
7	PdAu-5K-50AA (c)	50	5	74	32.5	15.9
8	PdAu-10K-50AA	50	10	73	62.5	32.3
9	PdAu-0K-100AA	100	0	79	22.5	7.4
10	PdAu-5K-100AA	100	5	76	25	11.6
11	PdAu-10K-100AA	100	10	68	57.5	28.4

Table S7. Pd-acetate responses from experimental design.

Run	Sample	AcOH (vol%)	K (wt%)	Integrated Intensity (cm ⁻¹)		
				Monodentate acetate on surface Pd	Pd ₃ (OAc) ₆	K ₂ Pd ₂ (OAc) ₆
1	PdAu-0K	0	0	0.00	0.00	0.00
2	PdAu-5K	0	5	0.00	0.00	0.00
3	PdAu-10K	0	10	0.81	5.55	0.00
4	PdAu-0K-50AA	50	0	0.00	0.61	0.53
5	PdAu-5K-50AA (a)	50	5	0.98	6.29	7.51
6	PdAu-5K-50AA (b)	50	5	1.28	6.31	7.50
7	PdAu-5K-50AA (c)	50	5	1.27	6.14	7.45
8	PdAu-10K-50AA	50	10	9.61	30.4	26.3
9	PdAu-0K-100AA	100	0	0.00	0.77	0.77
10	PdAu-5K-100AA	100	5	1.37	7.98	8.91
11	PdAu-10K-100AA	100	10	7.83	27.3	23.3

Table S8. Uncoded and coded parameters, *t*-values, and *p*-values of each effect for the Au grain size response curve.

Effect ^a	Uncoded parameters		Coded parameters		<i>t</i> -value	<i>p</i> -value
	Coeff.	SE	Coeff.	SE		
Constant	12.49	1.26	17.282	0.728	23.74	0.000
<i>A</i>	0.1307	0.0401	2.038	0.579	3.52	0.017
<i>B</i>	0.303	0.401	-0.508	0.579	-0.88	0.421
<i>AA</i>	-0.000571	0.000357	-1.426	0.892	-1.60	0.171
<i>BB</i>	-0.0076	0.0357	-0.190	0.892	-0.21	0.839
<i>AB</i>	-0.00658	0.00284	-1.644	0.710	-2.32	0.068

^a*A* is linear AcOH vol% effect, *B* is linear K wt% effect, *AA* is quadratic AcOH vol% effect, *BB* is quadratic K wt% effect, and *AB* is AcOH vol% and KOAc wt% interaction effect

Table S9. Uncoded and coded parameters, *t*-values, and *p*-values of each effect for the PdAu grain size response curve.

Effect ^a	Uncoded parameters		Coded parameters		<i>t</i> -value	<i>p</i> -value
	Coeff.	SE	Coeff.	SE		
Constant	8.206	0.131	8.4887	0.0753	112.71	0.000
<i>A</i>	0.01838	0.00415	0.1746	0.0599	2.91	0.033
<i>B</i>	-0.0990	0.0415	-0.0327	0.0599	-0.55	0.609
<i>AA</i>	-0.000145	0.000037	-0.3614	0.0922	-3.92	0.011
<i>BB</i>	0.00967	0.00369	0.2417	0.0922	2.62	0.047
<i>AB</i>	-0.000086	0.000294	-0.0214	0.0734	-0.29	0.782

^a*A* is linear AcOH vol% effect, *B* is linear K wt% effect, *AA* is quadratic AcOH vol% effect, *BB* is quadratic K wt% effect, and *AB* is AcOH vol% and KOAc wt% interaction effect

Table S10. Uncoded and coded parameters, *t*-values, and *p*-values of each effect for the Pd surface content response curve.

Effect ^a	Uncoded parameters		Coded parameters		<i>t</i> -value	<i>p</i> -value
	Coeff.	SE	Coeff.	SE		
Constant	79.58	1.28	74.100	0.740	100.17	0.000
<i>A</i>	-0.1045	0.0407	-2.250	0.589	-3.82	0.012
<i>B</i>	-0.095	0.407	-3.000	0.589	-5.10	0.004
<i>AA</i>	0.000980	0.000362	2.450	0.906	2.70	0.043
<i>BB</i>	-0.0120	0.0362	-0.300	0.906	-0.33	0.754
<i>AB</i>	-0.00770	0.00288	-1.925	0.721	-2.67	0.044

^a*A* is linear AcOH vol% effect, *B* is linear K wt% effect, *AA* is quadratic AcOH vol% effect, *BB* is quadratic K wt% effect, and *AB* is AcOH vol% and KOAc wt% interaction effect

Table S11. Uncoded and coded parameters, *t*-values, and *p*-values of each effect for the Pd²⁺ content response curve.

Effect ^a	Uncoded parameters		Coded parameters		<i>t</i> -value	<i>p</i> -value
	Coeff.	SE	Coeff.	SE		
Constant	-6.0	11.4	28.68	6.54	4.39	0.007
<i>A</i>	0.743	0.360	17.50	5.20	3.36	0.020
<i>B</i>	-0.32	3.60	16.25	5.20	3.12	0.026
<i>AA</i>	-0.00568	0.00320	-14.21	8.01	-1.77	0.136
<i>BB</i>	0.182	0.320	4.54	8.01	0.57	0.595
<i>AB</i>	0.0350	0.0255	8.75	6.37	1.37	0.228

^a*A* is linear AcOH vol% effect, *B* is linear K wt% effect, *AA* is quadratic AcOH vol% effect, *BB* is quadratic K wt% effect, and *AB* is AcOH vol% and KOAc wt% interaction effect

Table S12. Uncoded and coded parameters, *t*-values, and *p*-values of each effect for the monodentate acetate adsorbed on surface Pd response curve.

Effect ^a	Uncoded parameters		Coded parameters		<i>t</i> -value	<i>p</i> -value
	Coeff.	SE	Coeff.	SE		
Constant	-0.19	1.48	1.631	0.854	1.91	0.114
<i>A</i>	0.0579	0.0470	1.400	0.680	2.06	0.095
<i>B</i>	-0.740	0.470	3.041	0.680	4.47	0.007
<i>AA</i>	-0.000650	0.000418	-1.63	1.05	-1.55	0.181
<i>BB</i>	0.0997	0.0418	2.49	1.05	2.38	0.063
<i>AB</i>	0.00703	0.00333	1.757	0.832	2.11	0.089

^a*A* is linear AcOH vol% effect, *B* is linear K wt% effect, *AA* is quadratic AcOH vol% effect, *BB* is quadratic K wt% effect, and *AB* is AcOH vol% and KOAc wt% interaction effect

Table S13. Uncoded and coded parameters, *t*-values, and *p*-values of each effect for the Pd₃(OAc)₆ trimer response curve.

Effect ^a	Uncoded parameters		Coded parameters		<i>t</i> -value	<i>p</i> -value
	Coeff.	SE	Coeff.	SE		
Constant	-0.98	3.60	7.27	2.07	3.51	0.017
<i>A</i>	0.189	0.114	5.09	1.65	3.09	0.027
<i>B</i>	-1.67	1.14	10.32	1.65	6.26	0.002
<i>AA</i>	-0.00192	0.00101	-4.80	2.54	-1.89	0.117
<i>BB</i>	0.269	0.101	6.72	2.54	2.65	0.046
<i>AB</i>	0.02102	0.00808	5.26	2.02	2.60	0.048

^a*A* is linear AcOH vol% effect, *B* is linear K wt% effect, *AA* is quadratic AcOH vol% effect, *BB* is quadratic K wt% effect, and *AB* is AcOH vol% and KOAc wt% interaction effect

Table S14. Uncoded and coded parameters, *t*-values, and *p*-values of each effect for the $K_2Pd_2(OAc)_6$ dimer response curve.

Effect ^a	Uncoded parameters		Coded parameters		<i>t</i> -value	<i>p</i> -value
	Coeff.	SE	Coeff.	SE		
Constant	-1.21	3.69	8.41	2.12	3.96	0.011
<i>A</i>	0.211	0.117	5.50	1.69	3.25	0.023
<i>B</i>	-0.97	1.17	8.05	1.69	4.77	0.005
<i>AA</i>	-0.00213	0.00104	-5.34	2.60	-2.05	0.095
<i>BB</i>	0.145	0.104	3.63	2.60	1.40	0.221
<i>AB</i>	0.02253	0.00827	5.63	2.07	2.72	0.042

^a*A* is linear AcOH vol% effect, *B* is linear K wt% effect, *AA* is quadratic AcOH vol% effect, *BB* is quadratic K wt% effect, and *AB* is AcOH vol% and KOAc wt% interaction effect

Table S15. Uncoded and coded parameters, *t*-values, and *p*-values of each effect for the Pd loss response curve.

Effect ^a	Uncoded parameters		Coded parameters		<i>t</i> -value	<i>p</i> -value
	Coeff.	SE	Coeff.	SE		
Constant	-0.78	4.12	16.11	2.37	6.79	0.001
<i>A</i>	0.407	0.131	7.16	1.89	3.79	0.013
<i>B</i>	-0.42	1.31	8.36	1.89	4.42	0.007
<i>AA</i>	-0.00361	0.00116	-9.03	2.91	-3.11	0.027
<i>BB</i>	0.111	0.116	2.78	2.91	0.96	0.383
<i>AB</i>	0.01952	0.00925	4.88	2.31	2.11	0.089

^a*A* is linear AcOH vol% effect, *B* is linear K wt% effect, *AA* is quadratic AcOH vol% effect, *BB* is quadratic K wt% effect, and *AB* is AcOH vol% and KOAc wt% interaction effect

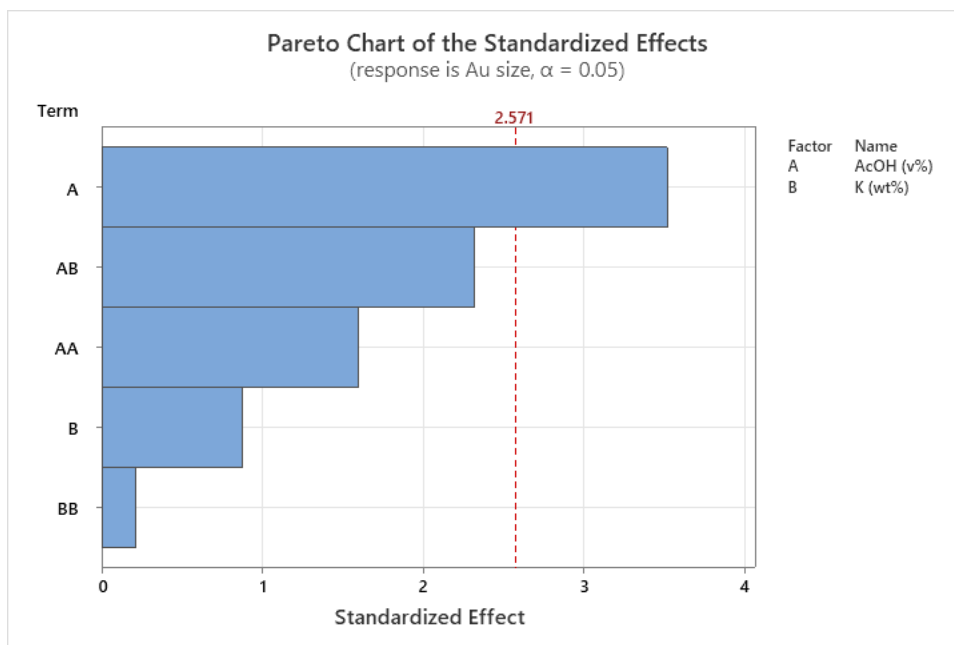


Figure S10. Pareto chart of standardized effects for Au grain size response where A is linear AcOH vol% effect, B is linear K wt% effect, AA is quadratic AcOH vol% effect, BB is quadratic K wt% effect, and AB is AcOH vol% and KOAc wt% interaction effect ($d.f. = 5$, $\alpha = 0.05$, $t_{sig} = 2.571$).

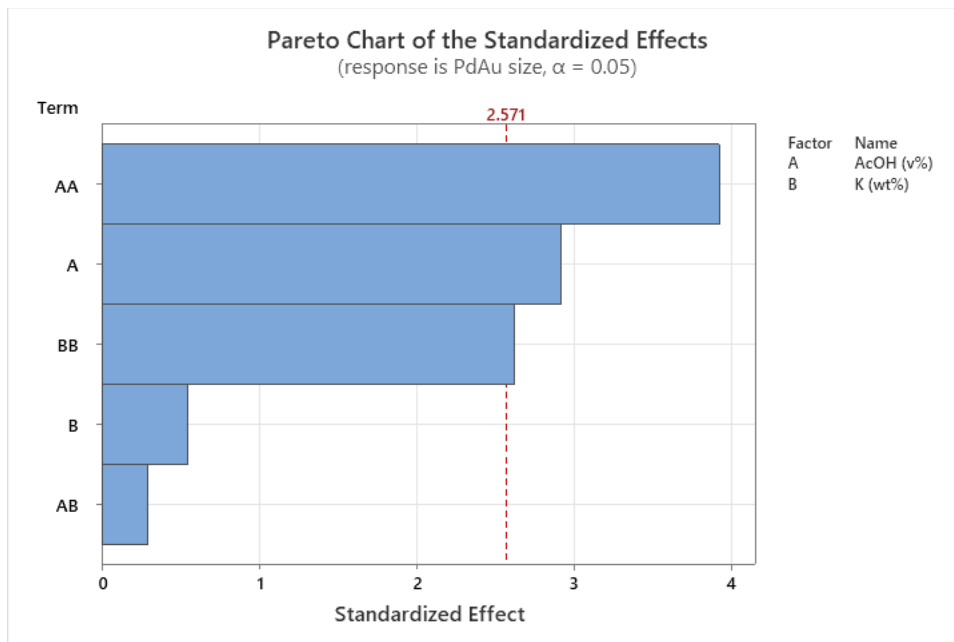


Figure S11. Pareto chart of standardized effects for Pd_xAu_y grain size response where A is linear AcOH vol% effect, B is linear K wt% effect, AA is quadratic AcOH vol% effect, BB is quadratic K wt% effect, and AB is AcOH vol% and KOAc wt% interaction effect ($d.f. = 5$, $\alpha = 0.05$, $t_{sig} = 2.571$).

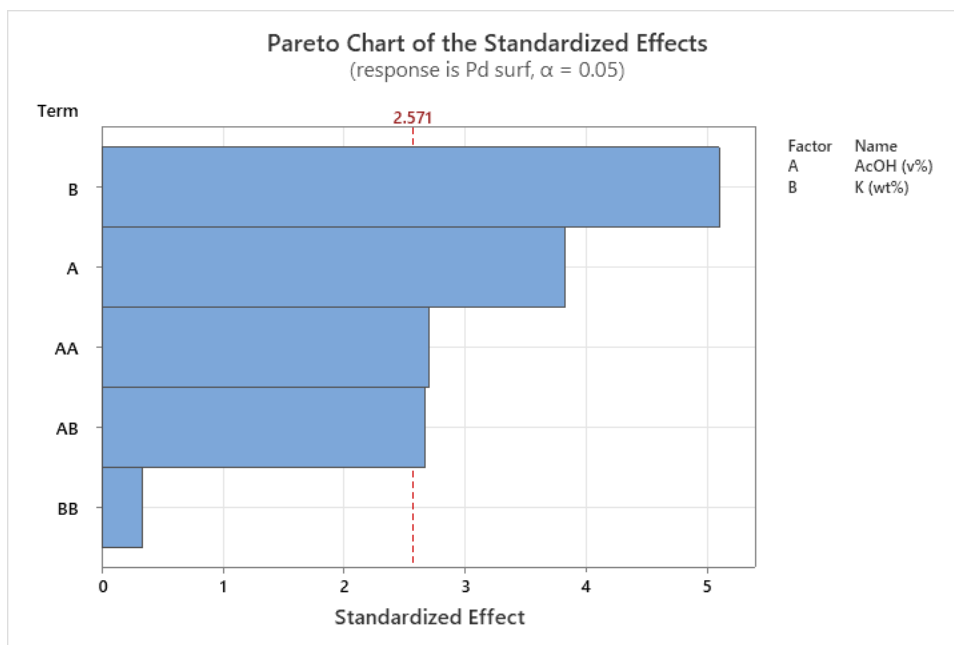


Figure S12. Pareto chart of standardized effects for Pd surface content response where A is linear AcOH vol% effect, B is linear K wt% effect, AA is quadratic AcOH vol% effect, BB is quadratic K wt% effect, and AB is AcOH vol% and KOAc wt% interaction effect ($d.f. = 5$, $\alpha = 0.05$, $t_{sig} = 2.571$).

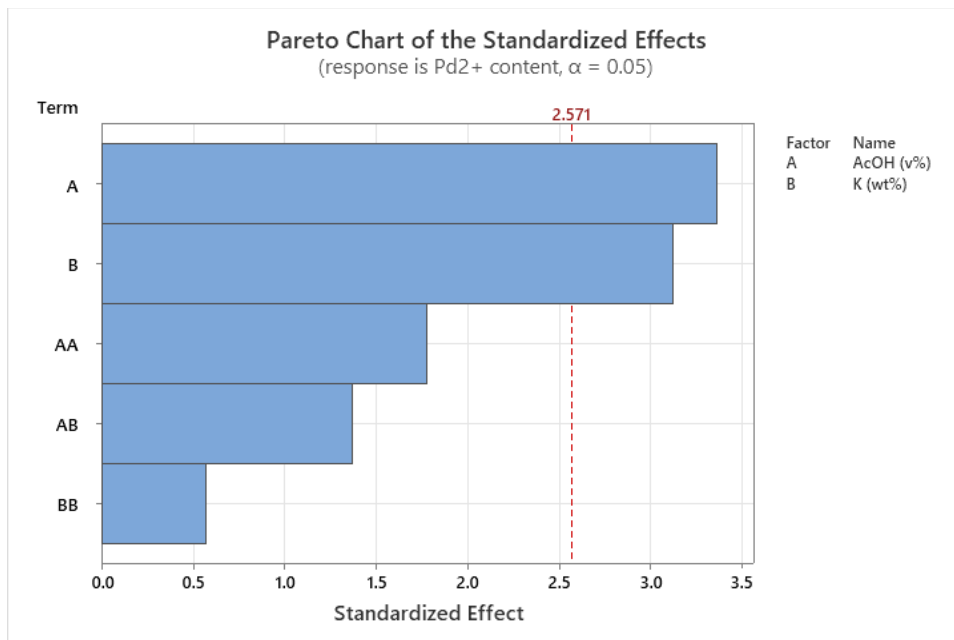


Figure S13. Pareto chart of standardized effects for Pd²⁺ content response where A is linear AcOH vol% effect, B is linear K wt% effect, AA is quadratic AcOH vol% effect, BB is quadratic K wt% effect, and AB is AcOH vol% and KOAc wt% interaction effect ($d.f. = 5$, $\alpha = 0.05$, $t_{sig} = 2.571$).

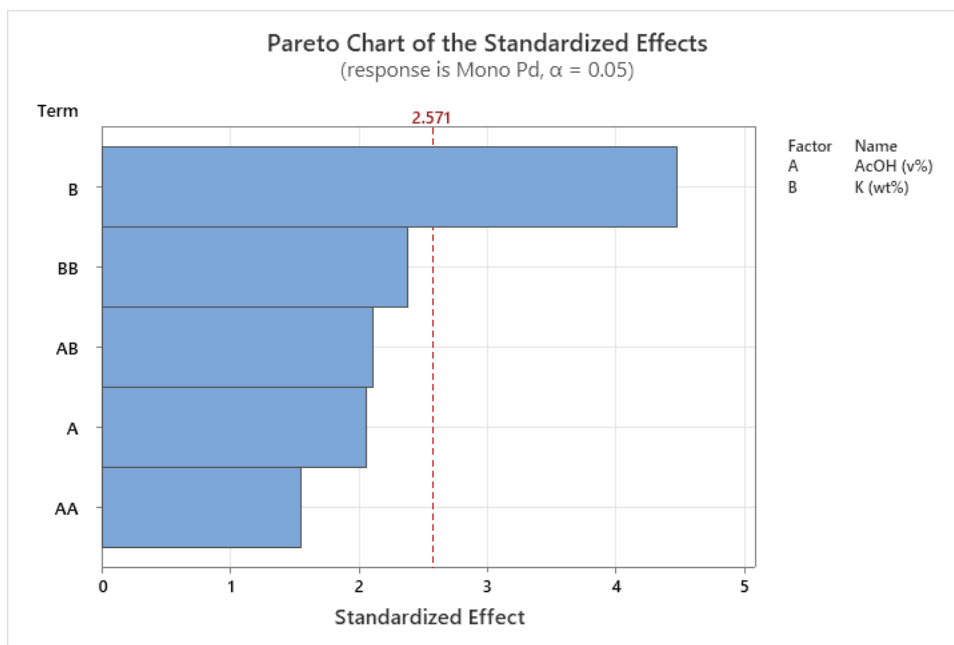


Figure S14. Pareto chart of standardized effects for moderate acetate adsorbed on surface Pd response where *A* is linear AcOH vol% effect, *B* is linear K wt% effect, *AA* is quadratic AcOH vol% effect, *BB* is quadratic K wt% effect, and *AB* is AcOH vol% and KOAc wt% interaction effect ($d.f. = 5$, $\alpha = 0.05$, $t_{sig} = 2.571$).

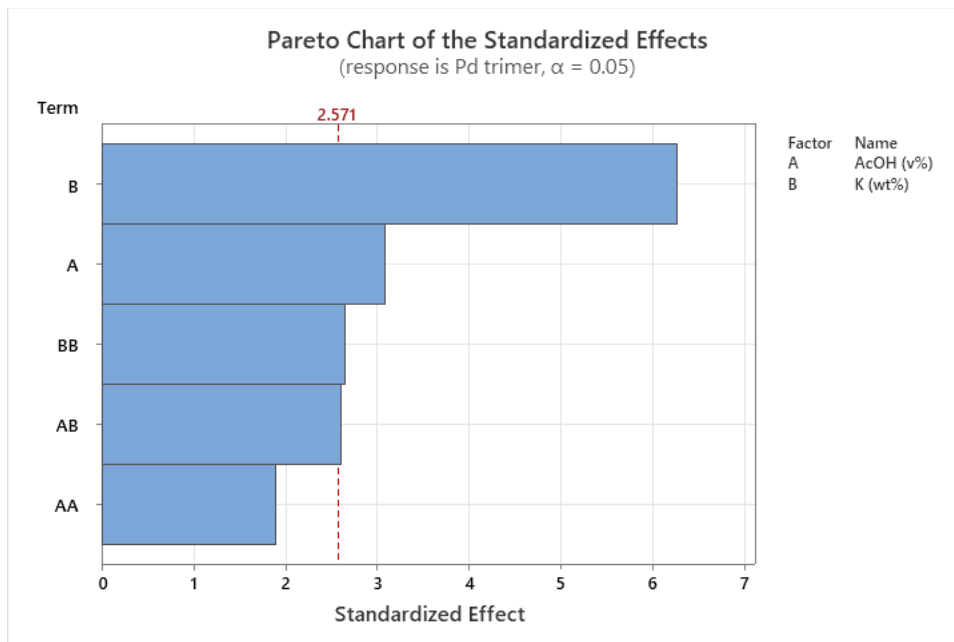


Figure S15. Pareto chart of standardized effects for $\text{Pd}_3(\text{OAc})_6$ response where *A* is linear AcOH vol% effect, *B* is linear K wt% effect, *AA* is quadratic AcOH vol% effect, *BB* is quadratic K wt% effect, and *AB* is AcOH vol% and KOAc wt% interaction effect ($d.f. = 5$, $\alpha = 0.05$, $t_{sig} = 2.571$).

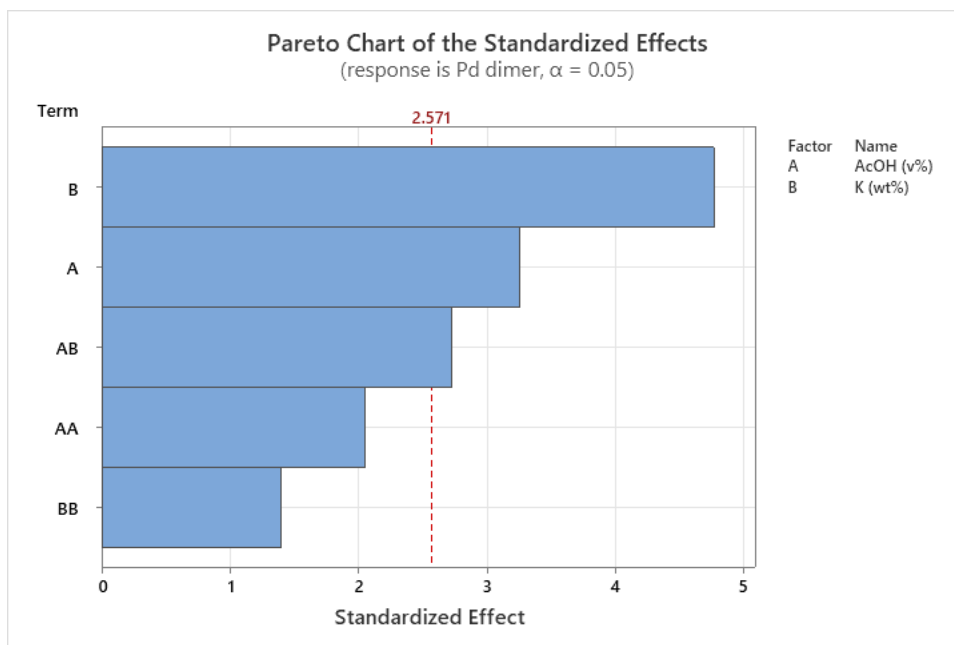


Figure S16. Pareto chart of standardized effects for $K_2Pd_2(OAc)_6$ response where A is linear AcOH vol% effect, B is linear K wt% effect, AA is quadratic AcOH vol% effect, BB is quadratic K wt% effect, and AB is AcOH vol% and KOAc wt% interaction effect ($d.f. = 5$, $\alpha = 0.05$, $t_{sig} = 2.571$).

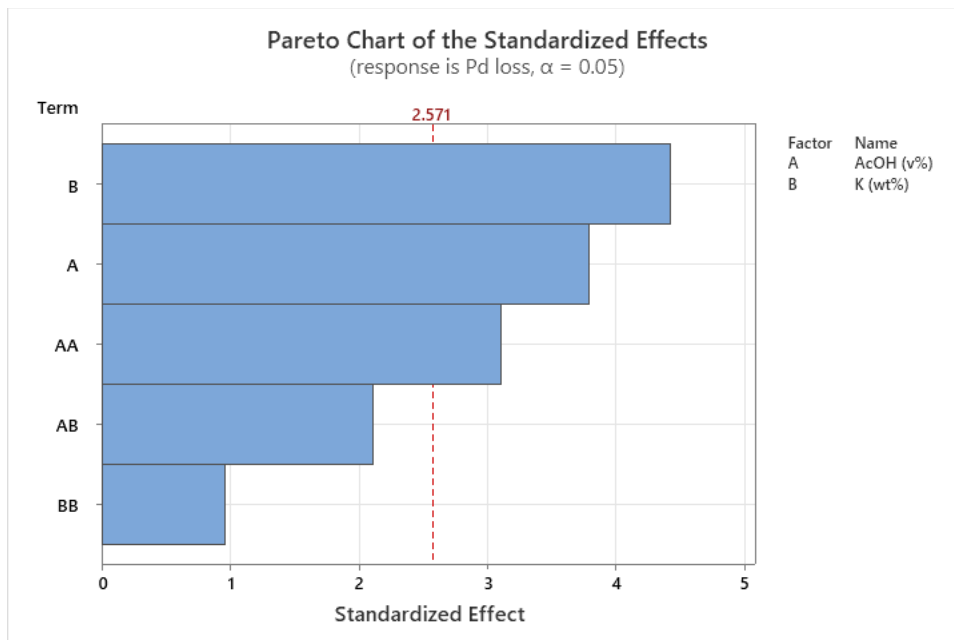


Figure S17. Pareto chart of standardized effects for Pd loss response where A is linear AcOH vol% effect, B is linear K wt% effect, AA is quadratic AcOH vol% effect, BB is quadratic K wt% effect, and AB is AcOH vol% and KOAc wt% interaction effect ($d.f. = 5$, $\alpha = 0.05$, $t_{sig} = 2.571$).