

Supporting Information

for

Surface functionalization of ZnO:Ag columnar thin films with AgAu and AgPt bimetallic alloy nanoparticles as an efficient pathway for highly sensitive gas discrimination and early hazard detection in batteries

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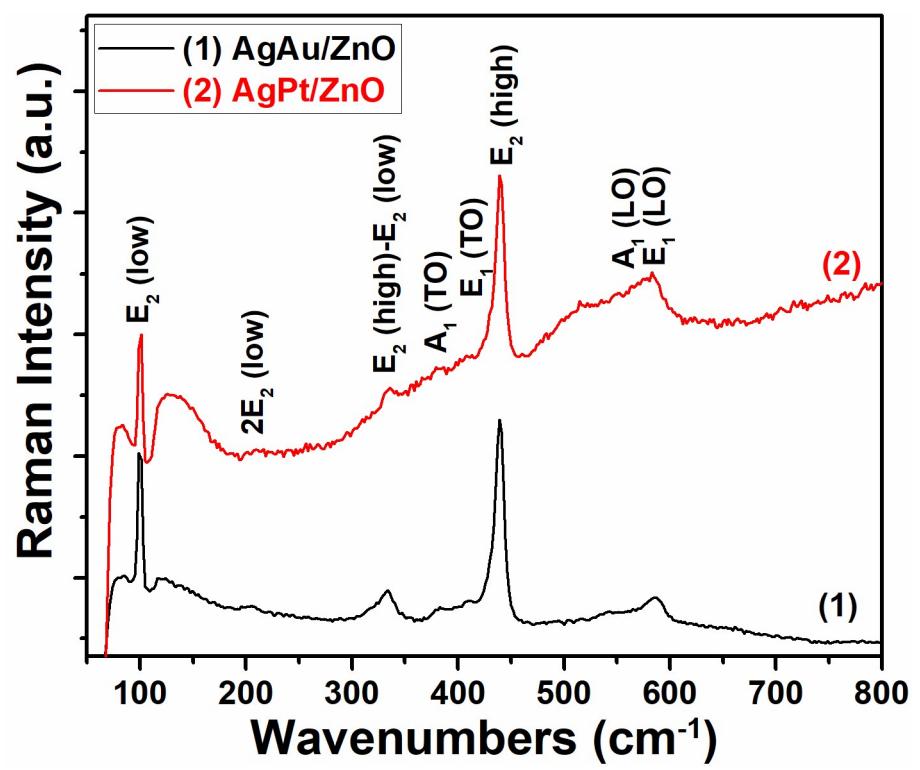


Figure S1. Room temperature Raman spectra of the AgAu- and AgPt-decorated ZnO:Ag columnar films.

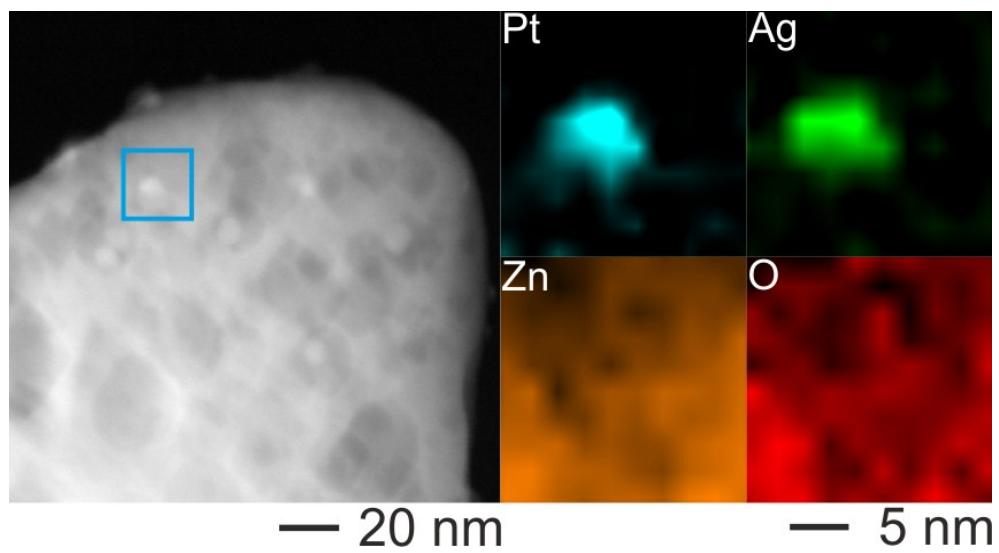


Figure S2. Left: Z-contrast STEM image showing a ZnO:Ag structure decorated with AgPt nanodots. Right: EDX elemental map of Ag and Pt distribution onto ZnO taken from the highlighted square region. The superimposed Ag and Pt distribution verifies the presence of AgPt alloy nanoparticles.

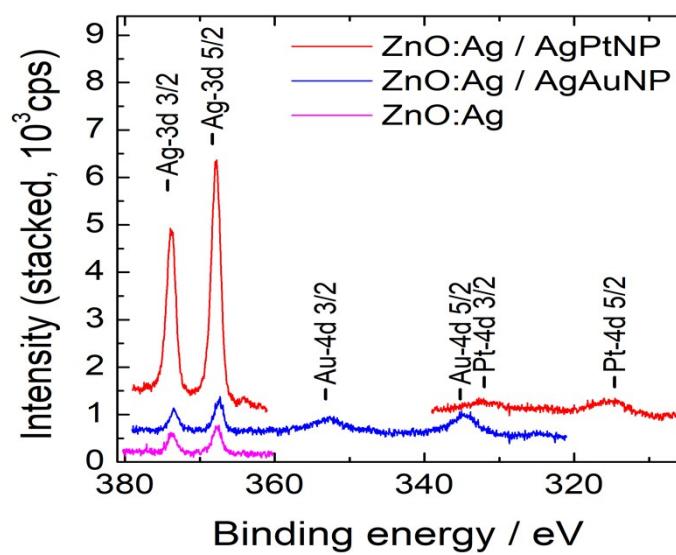


Figure S3. XPS spectra for the reference ZnO:Ag columnar thin film (magenta line), alloy NP decorated nanocomposites (AgAuNP: blue line) and (AgPtNP: red line); high resolution spectra of Ag-3d, Au-4d and Pt-4d lines.

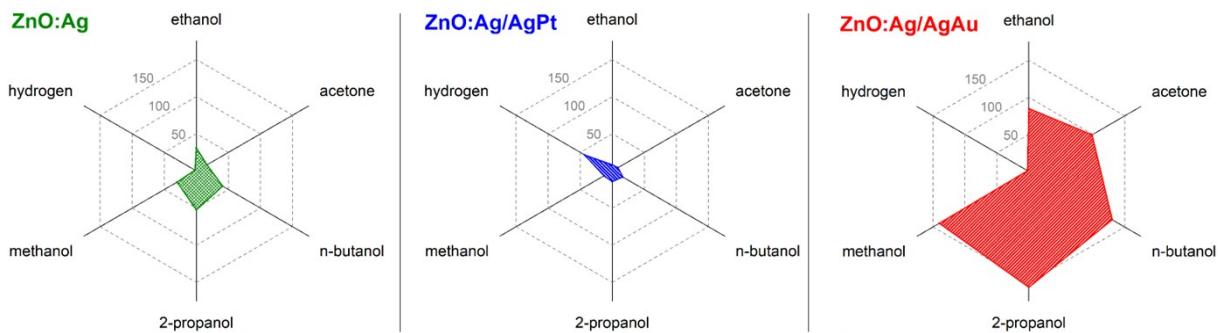


Figure S4. Gas response of ZnO:Ag thin film sensors can be significantly tailored upon surface decoration with noble metal alloy NPs, as shown by radar plots for an operating temperature of 250 °C. The pristine ZnO:Ag thin film sensor (green radar plot) exhibits considerable gas response to VOC vapors of ethanol, acetone, n-butanol, 2-propanol and methanol, while in comparison the gas response to H₂ is significantly lower. The AgAu/ZnO:Ag nanocomposite sensor (red radar plot) exhibits an enhanced sensitivity compared to the pristine ZnO:Ag thin film, while keeping a similar selectivity. In contrast, the AgPt/ZnO:Ag nanocomposite sensor (blue radar plot) shows a strong gas response towards H₂, while the gas response to all VOCs is drastically reduced compared to the ZnO:Ag and AgAu/ZnO:Ag sensors.

Table S1. Composition of AgPt and AgAu NPs as quantified by XPS.

Sample	Concentration of Pt	Concentration of Au	Concentration of Ag
AgPt/ZnO:Ag	~ 12% _{at}	-	~ 88% _{at}
AgAu/ZnO:Ag	-	~ 52% _{at}	~ 48% _{at}

Table S2. Summary of the unit cell parameters (a and c) of the hexagonal close packed (*hcp*) Zn, face-centred cubic (*fcc*) Ag, *fcc* Au and *fcc* Pt from this work and previous reports.

		a (Å)		c (Å)		
	Calculated	Experimental	Calculated	Experimental	Reference	
<i>hcp</i> Zn	2.650	2.664	4.528	4.946	1	
<i>fcc</i> Ag	4.140□□	4.086	—	—	2	
	□□□□□					
	□□□□□					
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<i>fcc</i> Au	4.234□□	4.071	—	—	3	
	□□□□□					
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<i>fcc</i> Pt	3.854□□	3.923	—	—	4	
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References

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