Electronic Supplementary Information

Fullerene Modification of Gold Electrodes and Gold Nanoparticles Based on Application of Aromatic Thioacetate-Functionalized C₆₀

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Figure S1. ESI-MS spectrum of 4-(S-acetylthio)benzaldehyde as a $[M + H]^+$ cation.



Figure S2. ESI-MS spectrum of aromatic thioacetate functionalized C_{60} fullerene (ATF- C_{60}) as a $[M+Na]^+$ cation.



Figure S3. ESI-MS spectrum of thiolate anion of deprotected ATF-C₆₀ as [M-H]⁻.



Figure S4. ESI-MS spectrum of *N*-acetylpyrrolidine present in methanol washings as $[M + H]^+$ cation.



Figure S5. IR spectrum of 4-(S-acetylthio)benzaldehyde in KBr disk.



Figure S6. IR spectrum of aromatic thioacetate functionalized C_{60} fullerene (ATF- C_{60}) in KBr disk.



Figure S7. ¹H NMR spectrum of 4-(S-acetylthio)benzaldehyde in CDCl₃.



Figure S8. ¹³C NMR spectrum of 4-(*S*-acetylthio)benzaldehyde in CDCl₃.



Figure S9. ¹H NMR spectrum of aromatic thioacetate functionalized C_{60} fullerene (ATF- C_{60}) in CDCl₃.



Figure S10. ¹³C NMR spectrum of aromatic thioacetate functionalized C_{60} fullerene (ATF-C₆₀) in CDCl₃.

	Size (d.nm):	% Volume:	St Dev (d.nm):
Peak 1:	4.716	100.0	1.210
Peak 2:	0.000	0.0	0.000
Peak 3:	0.000	0.0	0.000



Figure S11. Size distribution of synthesized bare octanethiol-AuNPs obtained from Dynamic

Light Scattering measurement.

	Size (d.nm):	% Volume:	St Dev (d.nm):
Peak 1:	301.2	0.2	62.91
Peak 2:	7.268	99.7	1.058
Peak 3:	106.9	01	19.67



Figure S12. Size distribution of AuNPs coated with fullerene derivative (**ATF-C**₆₀@AuNPs) obtained from Dynamic Light Scattering measurement.

Compound	C ₆₀	ATF-C ₆₀
E _{pc1} [V]	-0.467	-0.599
E _{pa1} [V]	-0.396	-0.522
E ₁ ^{0'} [V]	-0.432	-0.561
E _{pc2} [V]	-0.874	-0.951
E _{pa2} [V]	-0.807	-0.836
E ₂ ^{0'} [V]	-0.841	-0.894
E _{pc3} [V]	-1.40	-1.592
E _{pa3} [V]	-1.324	-1.573
E ₃ ^{0'} [V]	-1.362	-1.583
E _{pc4} [V]	-1.895	-2.099
E _{pa4} [V]	-1.828	-2.016
E4 ^{0'} [V]	-1.862	-2.013
E _{pc5} [V]	-2.417	a)
E _{pa5} [V]	-2.274	a)
E ₅ ^{0'} [V]	-2.346	a)

Table S1. Comparison of electrochemical properties of C_{60} and ATF- C_{60} CV and D	OPV (bottom)
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Compound	C ₆₀	ATF-C ₆₀
i _{c1} c ⁻¹ [Amol ⁻¹ dm ³]	1.57.10-2	8.49.10-3
i _{a1} c ⁻¹ [Amol ⁻¹ dm ³]	1.14.10-2	7.62.10-3
i _{a1} c ⁻¹ / i _{c1} c ⁻¹	0.73	0.90
i _{c2} c ⁻¹ [Amol ⁻¹ dm ³]	1.29.10-2	6.81·10 ⁻³
i _{a2} c ⁻¹ [Amol ⁻¹ dm ³]	1.21.10-2	6.7.10-3
$i_{a2}c^{-1}/i_{c2}c^{-1}$	0.94	0.973
i _{c3} c ⁻¹ [Amol ⁻¹ dm ³]	1.29.10-2	5.47.10-3
i _{a3} c ⁻¹ [Amol ⁻¹ dm ³]	1.21.10-2	6.86·10 ⁻³
$i_{a3}c^{-1}/i_{c3}c^{-1}$	0.94	0.79
i _{c4} c ⁻¹ [Amol ⁻¹ dm ³]	1.36.10-2	5.54·10 ⁻³
i _{a4} c ⁻¹ [Amol ⁻¹ dm ³]	1.10-2	1.14.10-2
i _{a4} c ⁻¹ / i _{c4} c ⁻¹	0.74	0.526

a) Peak corresponding to step 5 could not be resolved due to final rise of current

Compound	C ₆₀	ATF-C ₆₀
E ₁ [V]	-0.422	-0.559
_{b1/2} [mV]	103	107
E ₂ [V]	-0.827	-0.974
_{b1/2} [mV]	98	107
E ₃ [V]	-1.342	-1.550
_{b1/2} [mV]	98	103
E ₄ [V]	-1.845	-2.063
_{b1/2} [mV]	98	107
E ₅ [V]	-2.338	-
_{b1/2} [mV]	88	-
E ₆ [V]	-2.656	-
_{b1/2} [mV]	44	-