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Supporting Information

A strong linear correlation between the surface charge density on Ag nanoparticles and the amount of propylene adsorbed

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Table S1. Properties of Ag NPs depending on the TCNQ concentration

#	Applied TCNQ in solution [mol% to 100 mg Ag NPs]	Applied TCNQ in solution [µM]	Adsorbed TCNQ [µmol/ 100 mg Ag]	Surface coverage by TCNQ [%]	Adsorbed TCNQ [molecules/ nm^2]	Binding Energy of Ag (eV)	Propylene adsorption (µg/100 mg NP)
1	0	0	0.000	0	0.00	368.25	76.58
2	0.01	9	0.080	2.26	0.06	369.73	167.74
3	0.025	23	0.124	4.08	0.09	368.89	201.26
4	0.05	47	0.354	11.66	**0.26**	**369.20**	244.06
5	0.075	70	0.618	20.33	**0.46**	**369.19**	**268.77**
6	0.1	93	0.739	24.30	0.55	369.09	247.76
7	0.125	116	0.900	29.62	0.67	368.93	201.47
8	0.15	140	1.036	34.08	0.77	368.78	190.90
9	0.175	164	0.884	29.07	0.66	368.70	178.33
10	0.2	186	0.986	32.44	0.74	368.37	196.19

Table S2. Calculated adsorption energies (eV) of TCNQ and propylene adsorbed on the Ag(111) surface

Surface coverage by TCNQ (%)	TCNQ adsorption		TCNQ + propylene adsorption	
	Configuration	Adsorption energy (eV)	Configuration	Adsorption energy (eV)
0	(V-V-V-V)	-	(P-V-P-V)	-0.078
25	(T-V-V-V)	-0.427	(T-P-V-V)	-0.444
			(T-V-P-V)	-0.423
50	(T-T-V-V)	-0.643	(T-T-P-V)	-0.587
	(T-V-T-V)	-0.786	(T-P-T-V)	-0.750
			(T-P-T-P)	-0.885
			(P-V-P-V)	-0.026
75	(T-T-T-V)	-0.856	(T-T-T-P)	-0.885
100	(T-T-T-T)	-0.925	(P-P-P-P)	5.973
100 + 50	(T-T-T-T) + (T-V-T-V)	-0.036		
100 + 100	(T-T-T-T) + (T-T-T-T)	0.606		

V: Vacant, T: TCNQ and P: Propylene

+ represents the second layer

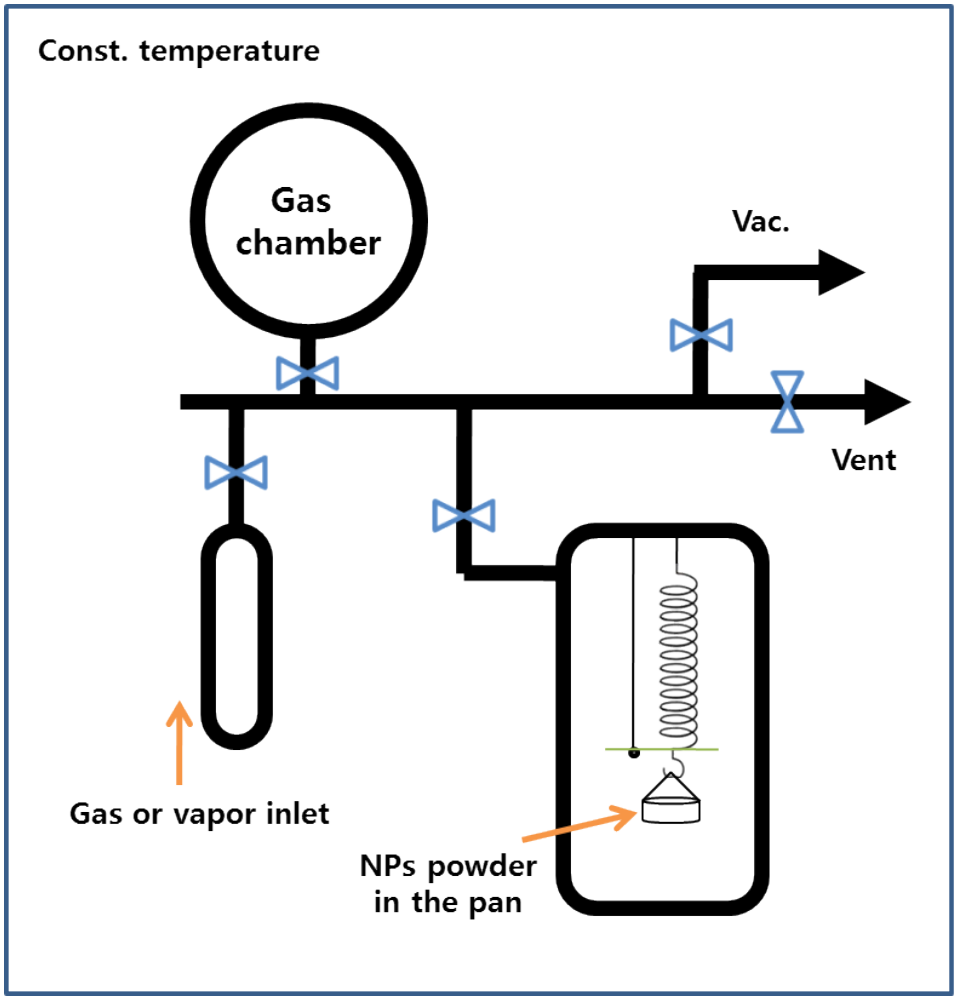

Figure S1. Schematic illustration of the sorption measurement equipment

The micro-change of Ag NPs weight upon propylene adsorption was measured by gravimetrical method, the extent of the stretched length of the quartz spring. First, the home-made instrument as depicted above (Figure S1) was set up and the constant temperature was maintained. The customized quartz spring was utilized to measure the weight change of the sample and the sample pan was made by Al foil to minimize the amount of gas absorption of the pan. The used quartz spring balance had a sensitivity of 100 μg/100 μm and was calibrated with a standard mass before use. The maximum weight and extension of the spring were 300.0 mg and 300.0 mm, respectively. Before the sorption measurement, (TCNQ-treated) Ag NPs sample was dried at vacuum condition. Then, the propylene or propane gas was applied to reach constant pressure. The propylene adsorption on the Ag NPs powder was calculated by measuring the position or length of the sample pan until the steady-state.

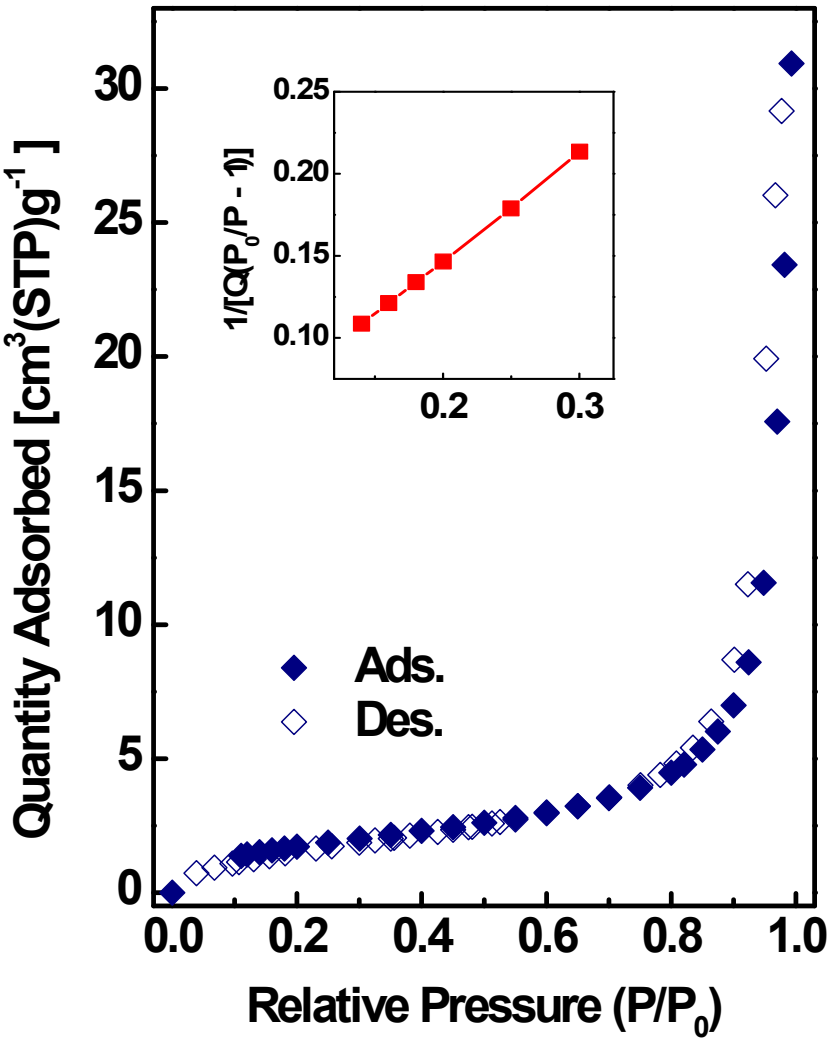

Figure S2. Isotherm adsorption of the NPs analysis by BET measurement

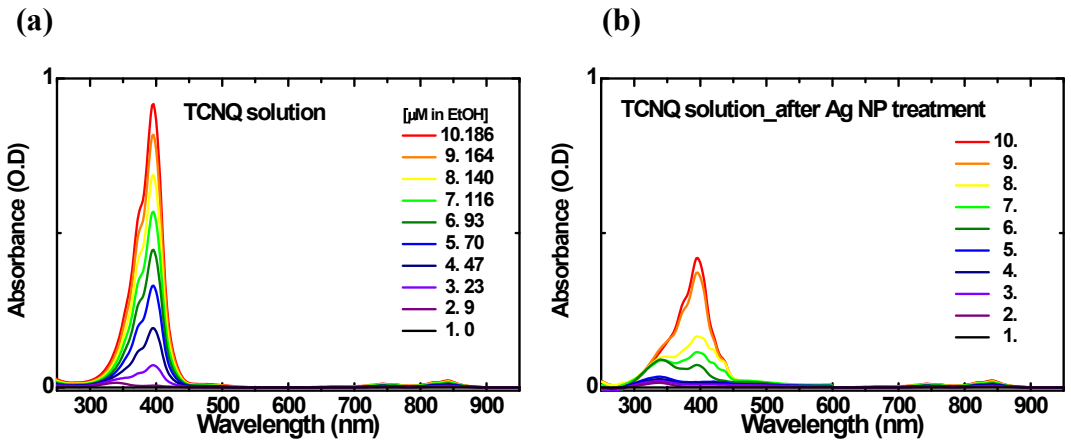

Figure S3. UV-Vis spectra of TCNQ solutions in ethanol upon changing the TCNQ concentr ation: (a) before and (b) after Ag NP immersion

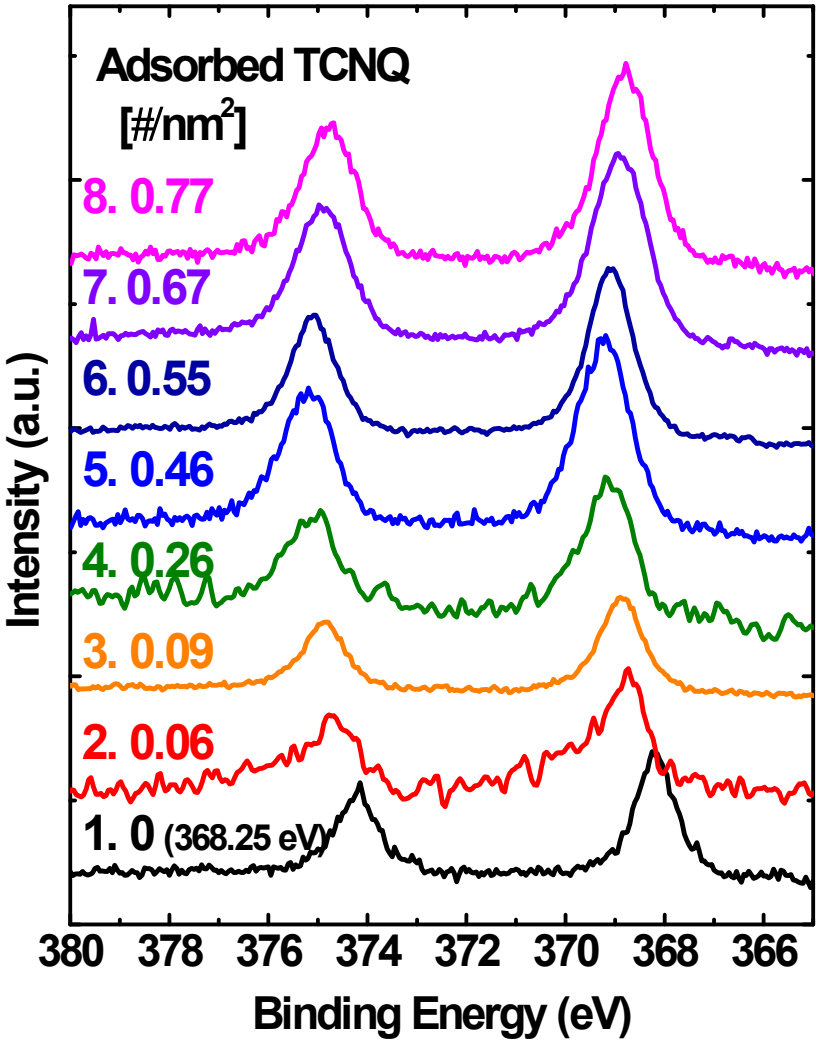

Figure S4. XPS spectra of Ag NPs adsorbed by various amounts of TCNQ molecules