surfaces

Supplementary Materials: Electrochemical Detection of Dinitrobenzene on Silicon Electrodes: Toward Explosives Sensors

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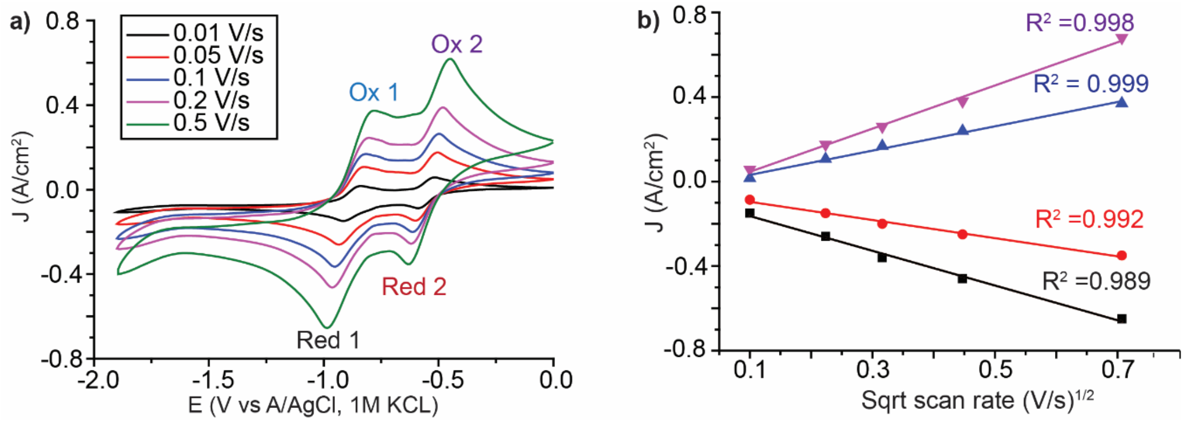

Figure S1. CV for 5 mM DNB on GCE. **a**) CV showing different scan rates for the GCE in 5 mM DNB solution. **b**) The correlation between the evolution of the peak current versus the scan rate showing a linear relationship between the square root (Sqrt) of the scan rate and the peak current, indicating that the redox process is diffusion-based electrochemical process.

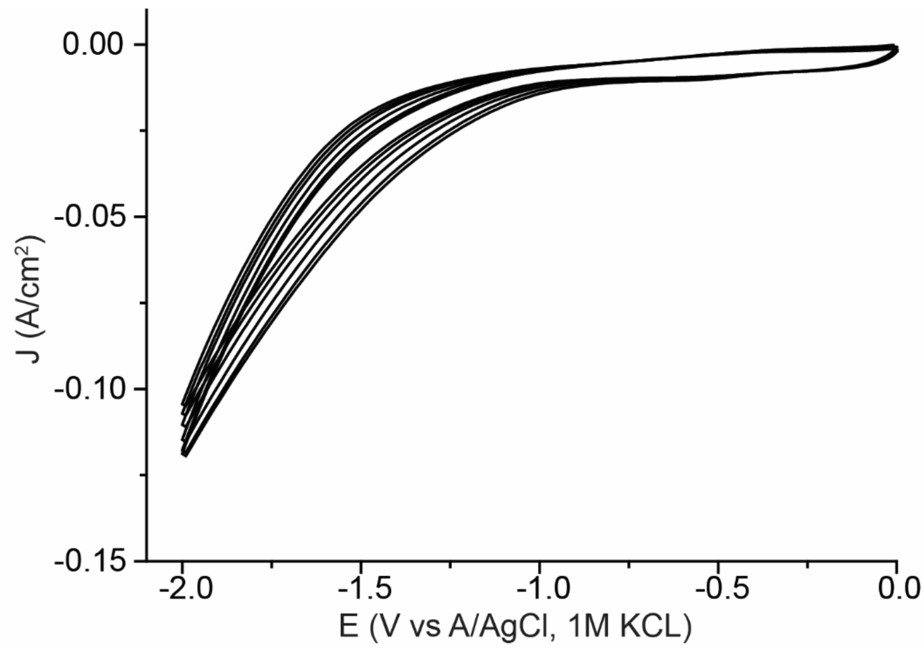

Figure S2. CV for GCE electrode in 0.5 M NBu_4PF_6 electrolyte in DMF, without DNB, at a scan rate of 0.1 $V{\cdot}s^{-1}$.

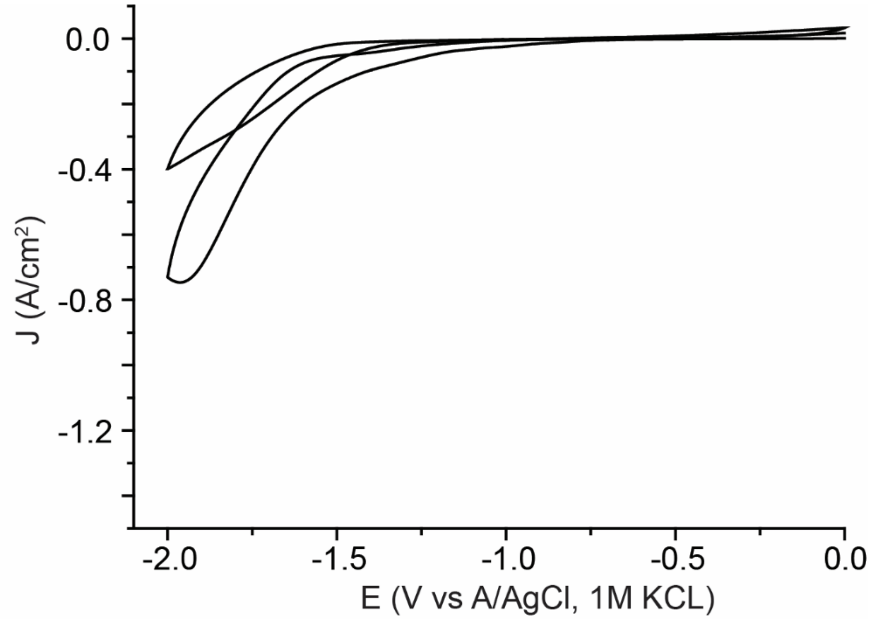

Figure S3. CV for Si–H surface in 0.5 M NBu_4PF_6 electrolyte in DMF, without DNB, at a scan rate of 0.1 V·s^{-1}.

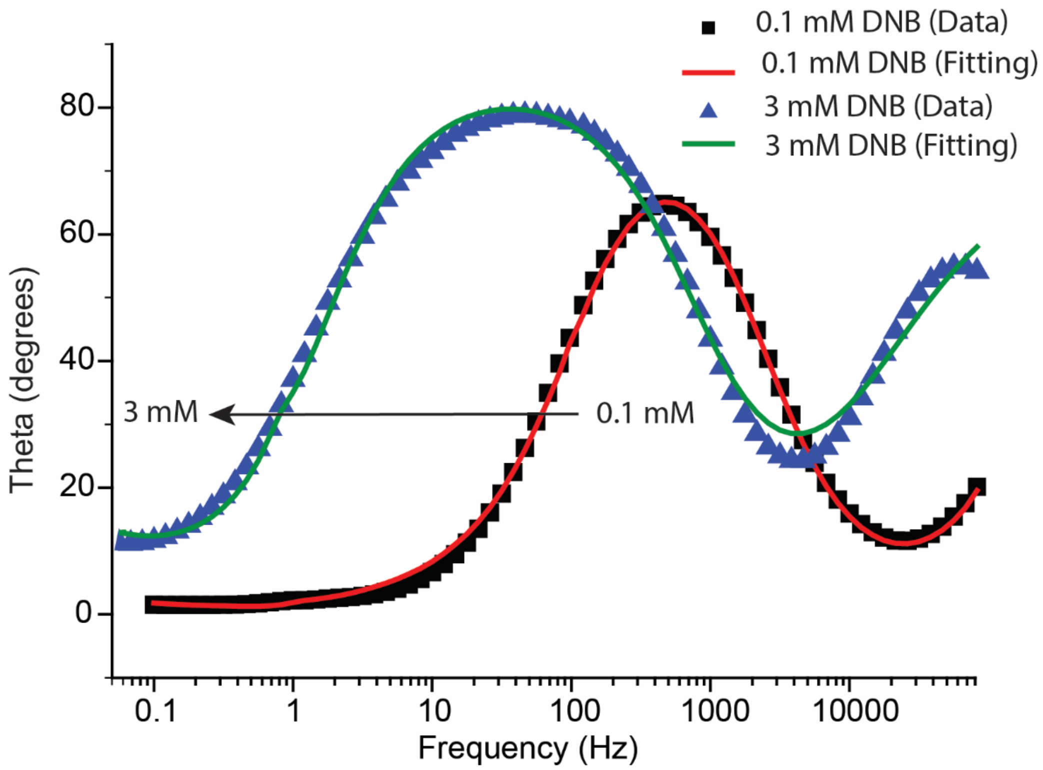

Figure S4. Bode plot for two different DNB concentrations, 0.1 mM (black dots represent raw data and red line represents the best fit of the Randles circuit) and 5 mM (blue dots represent raw data and green line represents the best fit of the Randles circuit), showing that the the phase angle valley shifts towards lower frequency with increasing concentration.

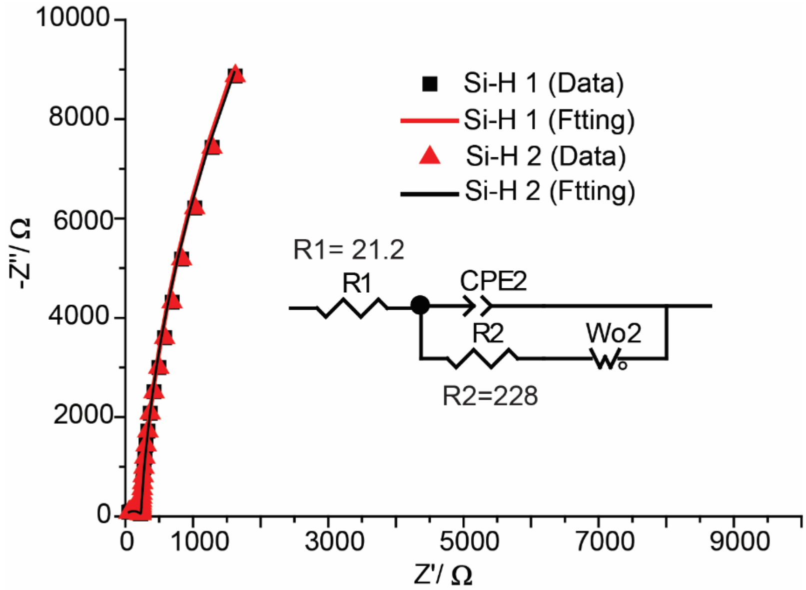

Figure S5. The equivalent Randles circuit used to fit the experimental EIS data. R1 represents the solution resistance, R2 represents the resistance of the free Si–H areas that are not covered by the polymer film, assuming that the polymer deposition occurs locally with a diffusion-controlled process, and CPE2 is a constant phase element that represents the capacitance over the area that is not covered by the polymer. R3 is the resistance of the polymer film or the area of the Si–H surface that is covered by the polymer, and CPE3 represents the capacitance of the polymeric film. Wo1 and CPE4 represent the Warburg diffusion element and the charging of the redox species in the electrolyte solution.

Table S1. Fitting parameters for the equivalent Randles circuit that was used to fit the Nyquist plots of the electrochemical impedance spectroscopy measured for the diffusion of the Ru $(NH3)_6{}^{3+/2+}$ ions through the DNB polymer films that were formed from using different concentrations of DNB. Each value is an average of three different measurements and the error represents the standard deviation from the averages.

DNB (mM)	R1 (Ω)	R2 (Ω)	CPE2 (F) (× 10^{-9})	R3 (Ω)	CPE3 (F) (× 10^{-7})	Wo-R	CPE4 (F)
0.01	12.01 ± 0.84	264.3 ±10.2	2.8 ± 0.3	1385 ± 233	5.1 ± 0.87	0.0015 ± 0.0002	0.0024 ± 0.0001
0.1	13.52 ± 0.92	205.5 ±8.1	3.7 ± 0.24	4993 ± 612	6.1 ± 1.1	0.0047 ± 0.0007	0.0018 ± 0.00015
1	12.8 ± 0.56	268 ± 10.5	3.6 ± 0.39	21,854 ± 3048	7.9 ± 0.92	5887 ± 753	0.0010 ± 0.00007
3	12.5 ± 0.71	255.3 ± 9.6	5.1 ± 0.27	44,785 ± 4089	8.5 ± 1.3	95,606 ± 6824	0.0001 ± 0.000016
20	12.62 ± 0.75	183.1 ± 6.5	2.7 ± 0.19	283,139 ± 16470	3.2 ± 0.52	115,294 ± 10651	0.0001 ± 0.00012

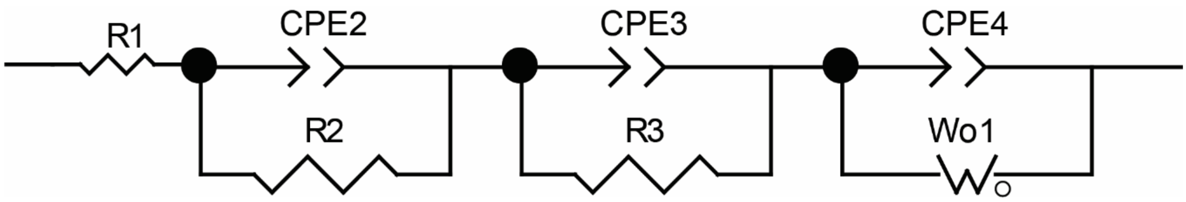

Figure S6. Nyquist plot fitted to a Randles circuit for Si–H electrode in 5 mM solution of hexamine ruthenium (III) chloride (in 50 mM KCl), without DNB reduction.

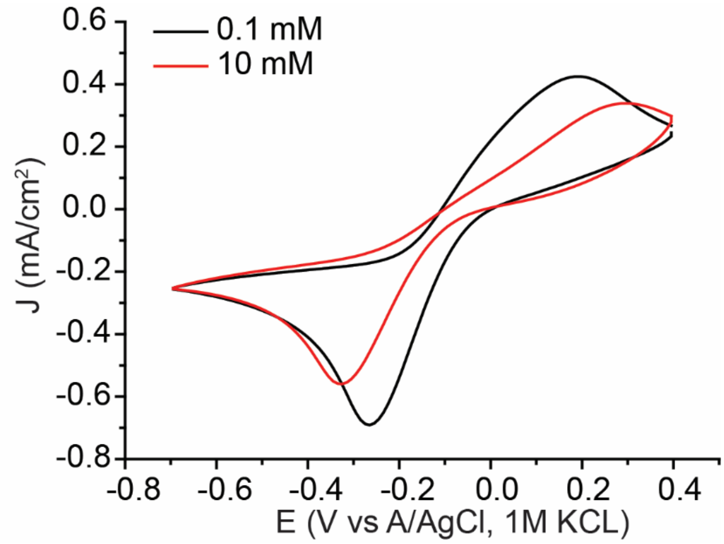

Figure S7. CV demonstrating the capability of the film in blocking the diffusion of Ru $(NH3)_6^{3+/2+}$ redox ions. The redox peaks are more separated, and the peak current intensity is inversely proportional to the concentration with 10 mM (red line) and 0.1 mM.