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Supplementary Information

Investigation of the Room Temperature Gas Sensing Properties of Metal-Organic Charge Transfer Complex $CuTCNQF_4$

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As-deposited $CuTCNF_4$ on alumina substrate

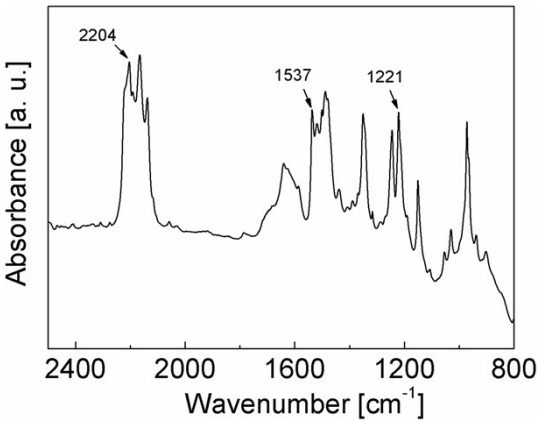

Fig. S1 FT-IR spectrum of as-deposited $CuTCNQF_4$ film.

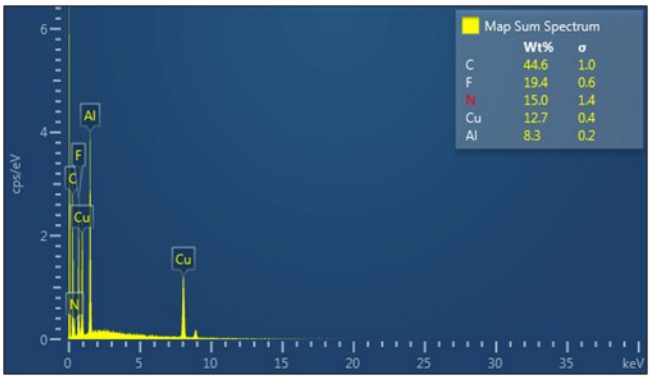

Fig. S2 EDX analysis of as-deposited $CuTCNQF_4$ film on alumina substrate.

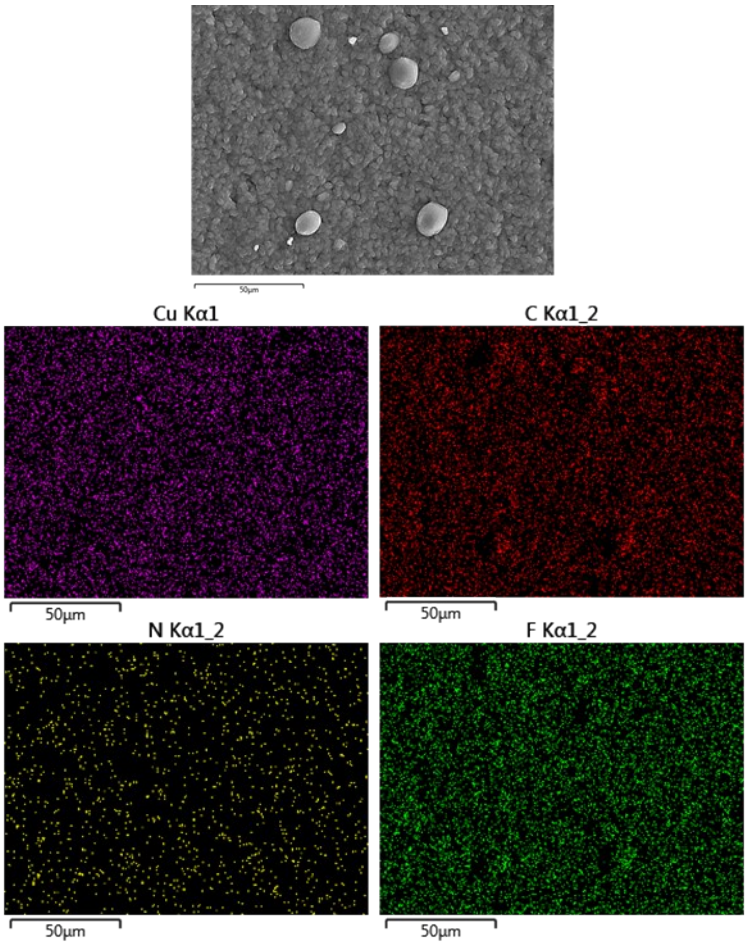

Fig. S3 SEM image and EDX mapping of as-deposited $CuTCNQF_4$ film on alumina substrate.

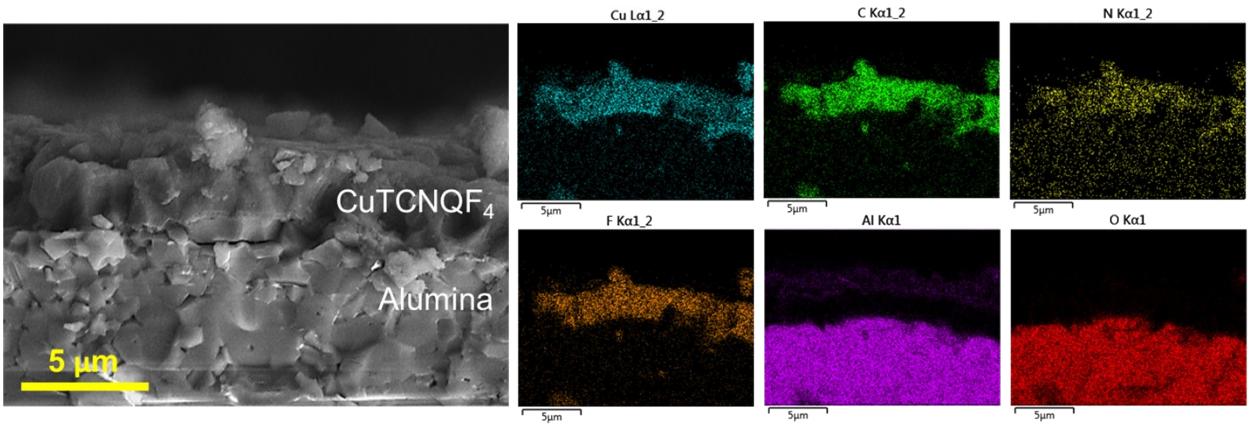

Fig. S4 SEM cross sectional image and EDX mapping of as deposited $CuTCNQF_4$ on alumina substrate.

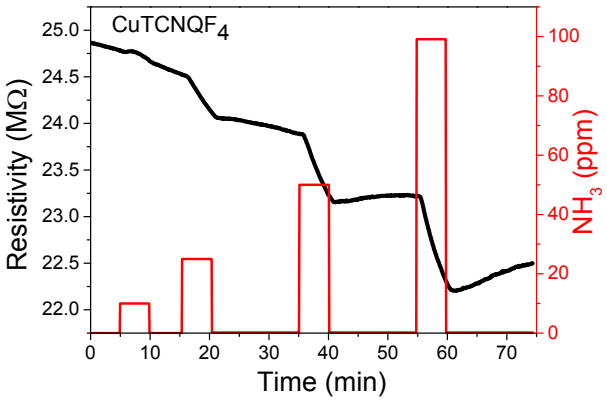

Fig. S5 Dynamic response of as-deposited $CuTCNQF_4$ film on alumina substrate towards NH_3 with different concentrations at 25°C.

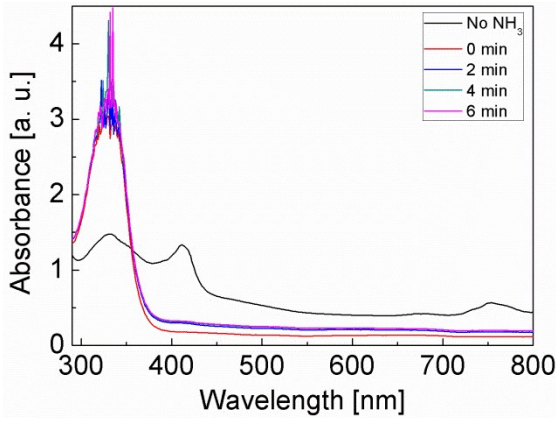

Fig. S6 Successive UV-vis absorption spectra of a solution obtained by dissolving $CuTCNQF_4$ in acetonitrile after adding NH_3 to the solution.

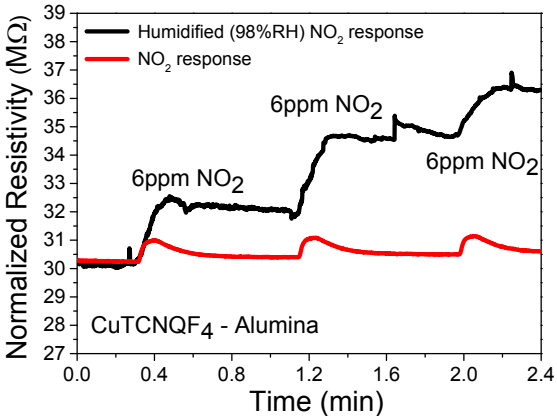

Fig. S7 Dynamic response of as-deposited $CuTCNQF_4$ film on alumina substrate towards dry and humidified NO_2 gas with 6 ppm concentration at 25°C.

As-deposited $CuTCNF_4$-Pt on alumina substrate

The $CuTCNQF_4$ film on the alumina substrate was decorated with Pt NPs via a simple galvanic replacement process. This approach was used previously to decorate CuTCNQ structures with Pt and Au nanoparticles and the galvanic replacement mechanism has been characterised in detail.[1-3] In a typical experiment, $CuTCNQF_4$ films were immersed in an aqueous solution of 1 mM K_2PtCl_4 for 18 h. Under these conditions there is enough thermodynamic driving force for $CuTCNQF_4$ to be oxidised to Cu^+ and $TCNQF_4^0$, donating electrons to the $PtCl_4^{2-}$ ions to form Pt nanoparticles on the surface of the film. Any neutral $TCNQF_4$ would then react with Cu generated via the disproportionation of Cu^+ in water to Cu^0 and Cu^{2+} ions to regenerate $CuTCNQF_4$ via the reaction of Cu^o and $TCNQF_4^0$, and therefore create a Pt decorated $CuTCNQF_4$ surface which is analogous to the metal nanoparticle decorated CuTCNQ system.[2]

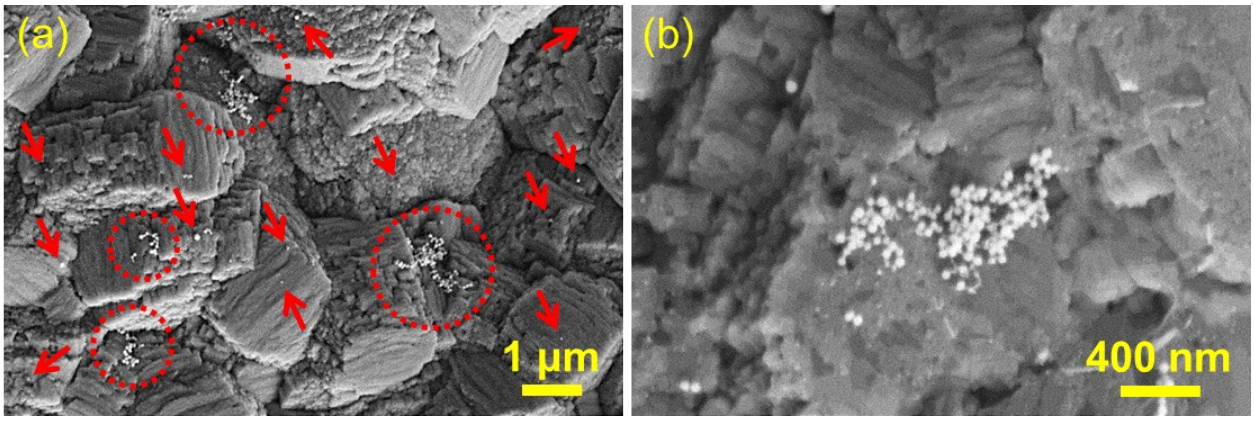

Fig. S8 (a) Overview and (b) higher resolution FESEM images of as-deposited $CuTCNQF_4$-Pt composite film. Arrows in (a) show the location of the Pt nanoparticles.

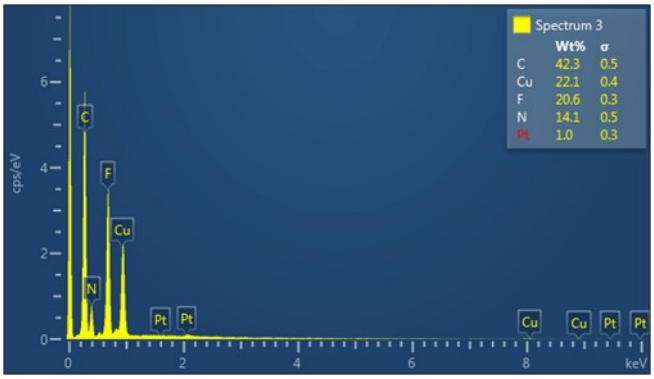

Fig. S9 EDX analysis of $CuTCNQF_4$-Pt film.

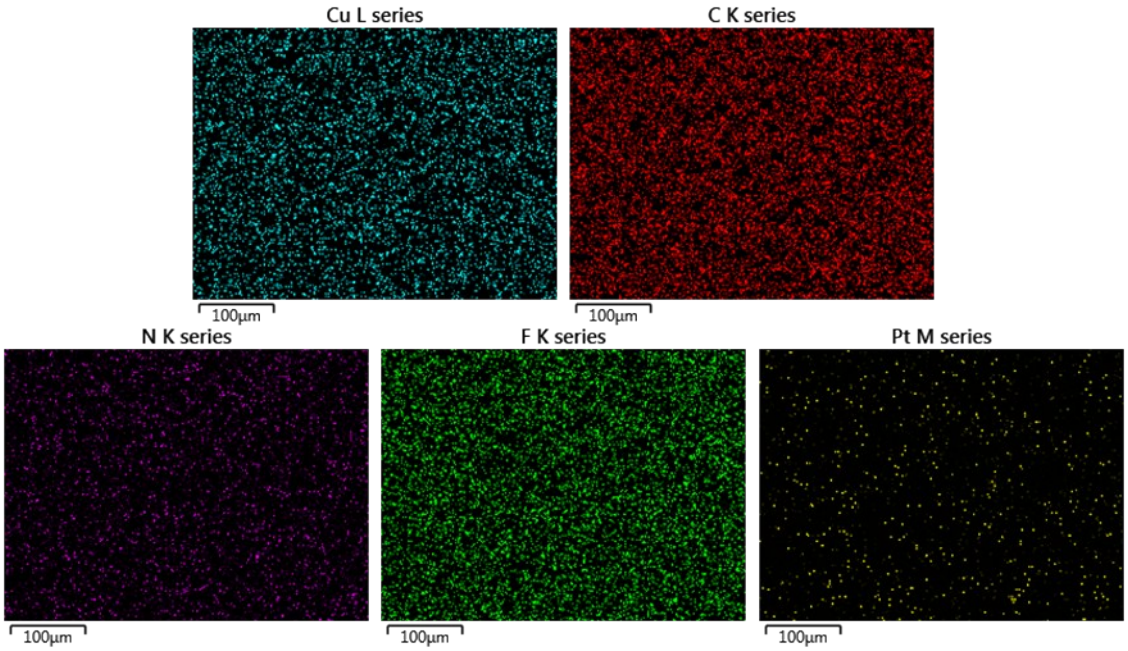

Fig. S10 EDX mapping of $CuTCNQF_4$-Pt film.

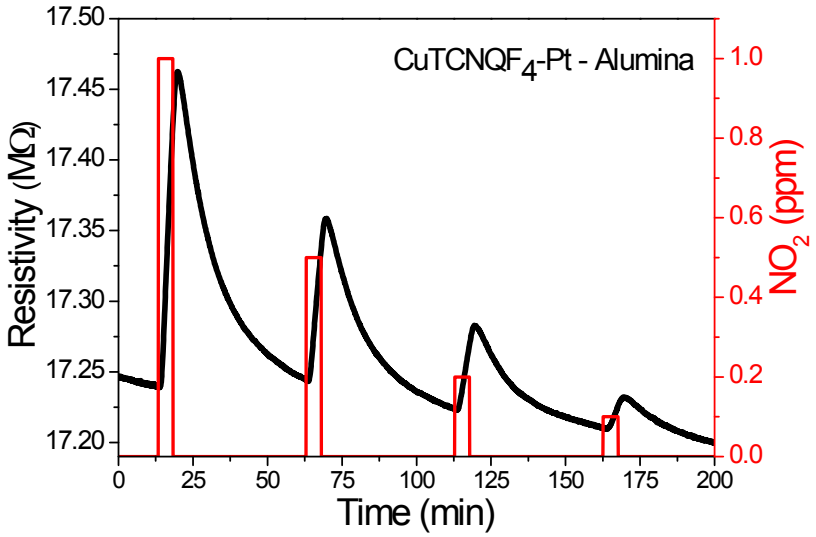

Fig. S11 Dynamic response of the as-deposited $CuTCNQF_4$-Pt film on alumina substrate towards NO_2 with concentrations in the range of 0.1-1 ppm at 25°C.

Table S1. Comparison between responses of as-deposited $CuTCNQF_4$ and $CuTCNQF_4$-Pt films on alumina substrate towards NO_2 at 25°C.

	Response to NO_2 (%)			
	0.1 ppm	**0.25 ppm**	**0.5 ppm**	**1 ppm**
$CuTCNQF_4$	0.133	0.27	0.51	0.99
$CuTCNQF_4$-Pt	0.12	0.34	0.66	1.23

References

1. A. Pearson and A. P. O'Mullane, *ChemPlusChem*, 2013, **78**, 1343-1348.
2. A. Pearson, A. P. O'Mullane, S. K. Bhargava and V. Bansal, *Inorg. Chem.*, 2012, **51**, 8791-8801.
3. A. Pearson, A. P. O'Mullane, V. Bansal and S. K. Bhargava, *Inorg. Chem.*, 2011, **50**, 1705-1712.