SUPPLEMENTARY INFORMATION

Structure Determination of F_4TCNQ on Ag(111): a Systematic Trend in Metal Adatom Incorporation

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NIXSW

Figure S1 shows the experimental NIXSW absorption profiles together with the best-fit results corresponding to the coherent fraction and position values reported in Table 1 of the main manuscript.

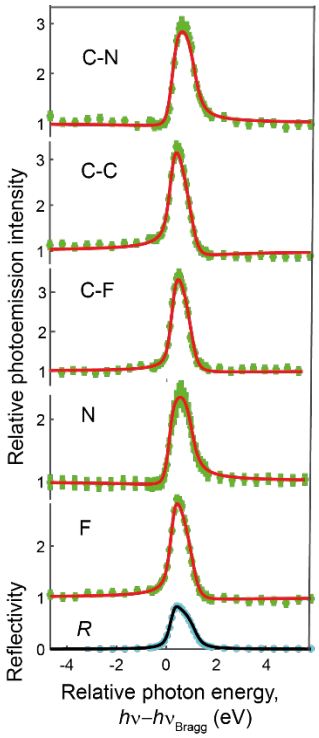

Figure S1 individual C 1s, N 1s and F 1s experimental NIXSW profiles (green data points) and best-fit theory curves (red lines) corresponding to the coherent fraction and coherent position values reported in Table 1. Also shown is the reflectivity, *R*.

Figures S2 and S3 shows comparisons of the experimental CTRs and FORs, respectively, with the results of simulations for the best-fit adatom and best-fit no adatom structural models.

SXRD

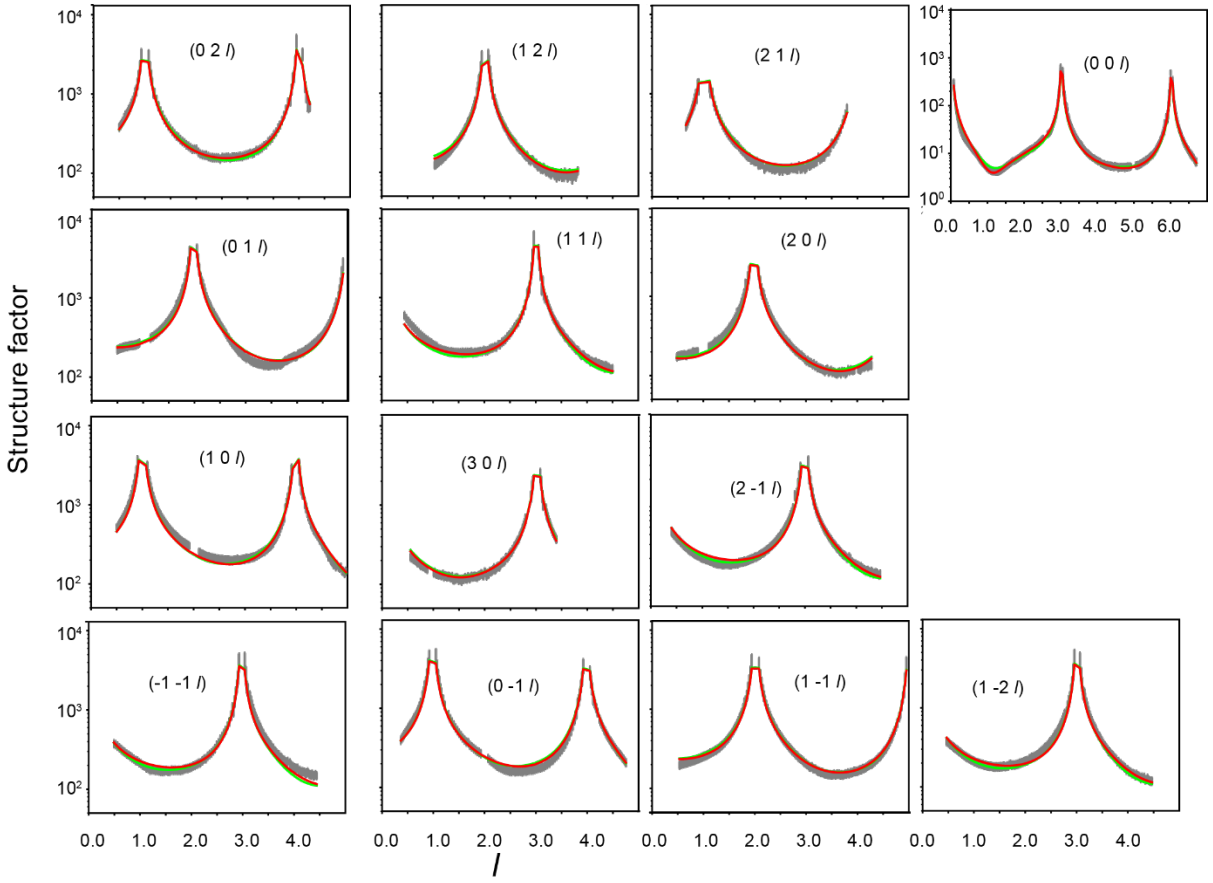

Figure S2 Experimental CTRs (grey data points) compared with the results of simulations for the best-fit adatom model (red curves) and the best-fit no-adatom model (green curves).

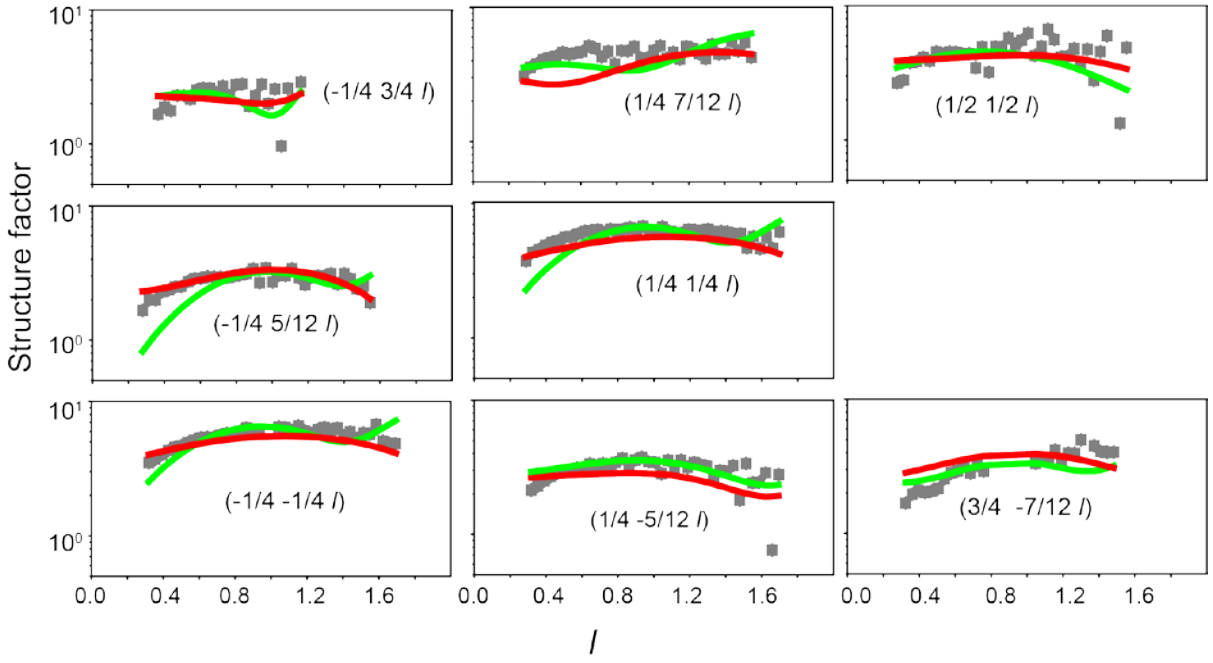

Figure S3 Experimental FORs (grey data points) compared with the results of simulations for the best-fit adatom model (red curves) and the best-fit no-adatom model (green curves).

Two-adatom structural model

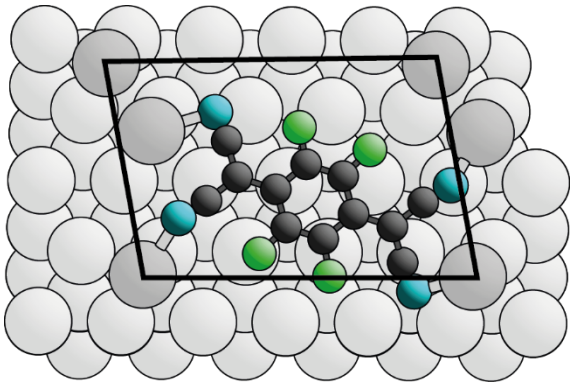

Figure S4 Plan view of the two-adatom model of the Ag(111) $\begin{bmatrix} 4 & 0 \\ 1 & 3 \end{bmatrix}$$F_4TCNQ$ structure giving the lowest value of χ^2 by SXRD. Atom colouring as in Figure 6 of the main manuscript.