Supplementary Material: Controlled low dimensionality in hybrid organic-inorganic superlattices

One-dimensional electron density map calculated from XRD results

X-ray diffraction spectrum reflects the electronic and atomic structure information of the material, which can be reversed from the XRD results.

The electron density along the c-axis could be obtained by

$$\rho\,(z) = \sum_{j=1}^{\infty} F_{00l} \cos\left(\frac{2\pi l z}{c}\right) \tag{S1}$$

where l, F_{00l}, and c represents the Miller index of the (00l) crystal plane, structure factor of the 00l reflections, and the interlayer distances, respectively.

The structure factors of the 00l reflections F_{00l} were derived from their intensities corrected for Lorentz-polarization effects

$$|F_{00l}| = (I/Lp)^{1/2} \tag{S2}$$

where I is the intensity of the peak intensity and L_p is the Lorentz-polarization factor which can be written as

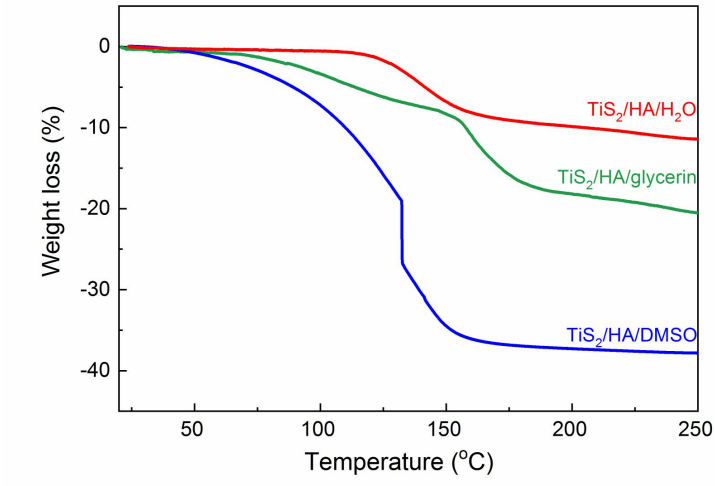
$$\mathrm{Lp} = (1 + \cos^2 2\theta)\big/(\sin^2\theta \cos\theta) \tag{S3}$$

The absolute values for F_{00l} can be derived by Eq. (4). The signs (phase) of the structure factor can be directly obtained instead from the scattering contributions of the inorganic atoms framework by assuming that the contribution from the intercalated organic molecules is relatively small.

$$F_{00l} = \sum_{j=1}^{N} 2f_i \cos(2\pi l z_i) \quad \text{(S4)}$$

where f_i is the scattering factor of j atom, z_i is its fractional coordinate on the c axis. Using Eq. (5), the sign for each F_{00l} was determined and combined with the absolute value in Eq. (4), and the one dimensional electron density map can be derived.

TGA result



Supplementary Figure 3. TGA result of hybrid inorganic-organic superlattices.