

Supplementary information for *Soft Matter* Manuscript:

Generic packing motifs in vapor-deposited glasses of organic semiconductors

Kushal Bagchi^a, Ankit Gujral^a, MF Toney^b, MD Ediger^a

^aDepartment of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53706, United States.

^bStanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, California 94025, United States.

(i) Regions of reciprocal space used for order parameter analysis.

Calculation of the order parameter requires an appropriate subtraction of background scatter. We calculate the order parameter from a narrow range of Q values near the peak scattering intensity. To determine the region in reciprocal space appropriate for evaluating the order parameter, first, the peak position along Q (in a $I(Q)$ vs Q plot) was determined, by summing over the entire accessible angular range. An example of such a plot, along Q , obtained by summing over the entire accessible angular range is shown in Fig S1, for an *m*-MTDATA glass prepared at $T_{\text{sub}}=260$ K. The region in reciprocal space used to evaluate the order parameter is shown in Fig S1. The upper and lower limits of the region used for the evaluation are chosen such that $Q_{\text{peak}} \sim (Q_{\text{min}} + Q_{\text{max}})/2$. A slice of the same width was chosen 0.6 \AA^{-1} away from the peak to estimate the background contribution to the scattered intensity. The background region is chosen such that the glass does not exhibit any diffraction peak in that region.

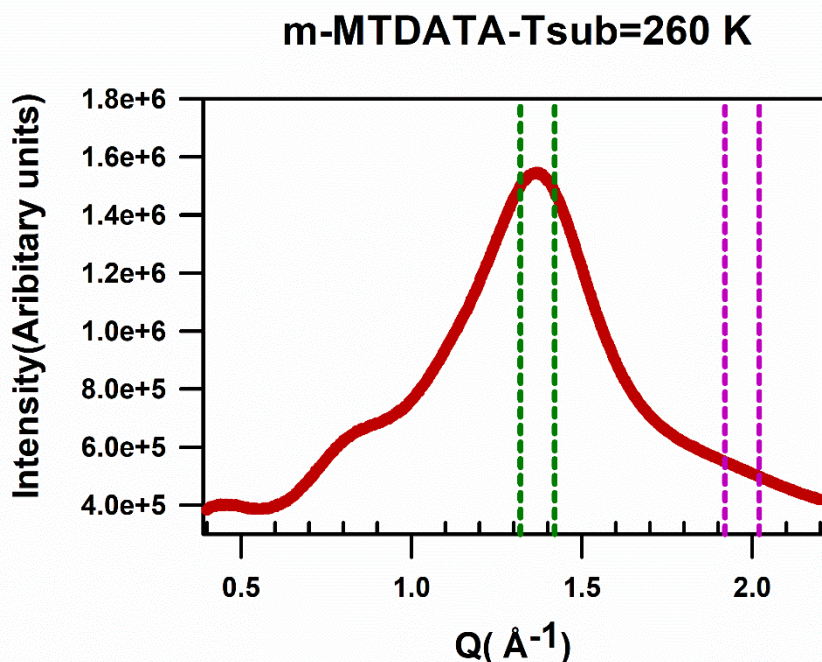


Fig S1: The intensity as a function of Q for a *m*-MTDATA glass prepared at $T_{\text{sub}}=260$ K, obtained by summing over the entire accessible angular range. The dashed green lines indicate the upper and lower limits of the region used to calculate the order parameter. The dashed purple lines indicate the upper and lower limits of the region in reciprocal space used to evaluate the background contribution.

After these two regions in Q space are identified, an angular distribution of scattering intensity is obtained by summing over Q at each angle. The “background” $I(\chi)$ vs χ curve is then subtracted from the “raw signal” $I(\chi)$ vs χ curve as shown in Fig S2. The background subtracted $I(\chi)$ vs χ curve is then used to calculate the order parameter as specified in equation 1 and 2 of the manuscript (note that the order parameter calculation *does* incorporate a sine correction). Shown below is an example of how the curve for order parameter calculations was obtained.

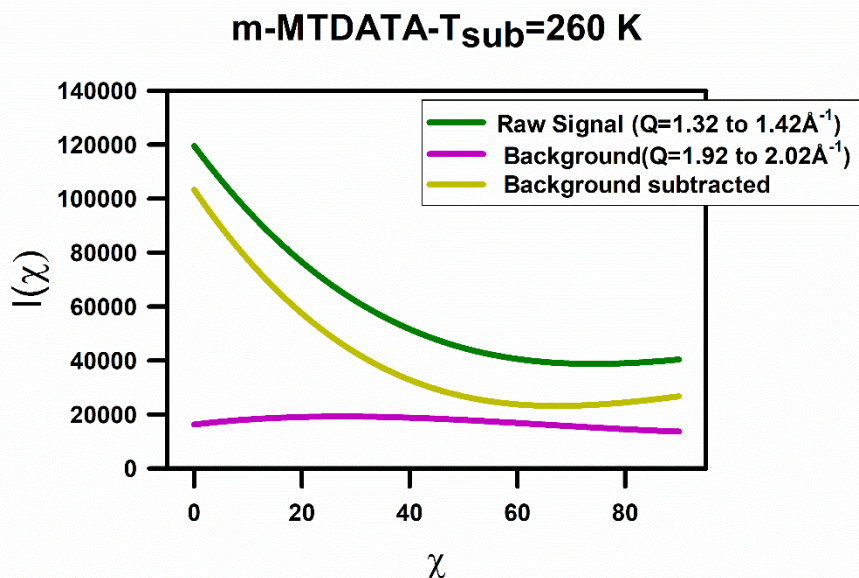


Fig S2: Shown are the angular distribution of scattering intensity for the “raw signal”, the “background curve” and for the background subtracted curve. The background subtracted curve is used for order parameter calculations.

This process is repeated for glasses of all the molecules. The regions in reciprocal space used to evaluate the raw signal and the background for glasses of all the molecules is shown in Table 1.

Table 1:

Molecule	Raw Signal(Q_{\min} to Q_{\max})	Background(Q_{\min} to Q_{\max})
DSA-Ph	1.35 to 1.45 \AA^{-1}	1.95 to 2.05 \AA^{-1}
m-MTDATA	1.32 to 1.42 \AA^{-1}	1.92 to 2.02 \AA^{-1}
TPD	1.34 to 1.44 \AA^{-1}	1.94 to 2.04 \AA^{-1}
Alq3	1.57 to 1.67 \AA^{-1}	2.17 to 2.27 \AA^{-1}
TCTA	1.40 to 1.50 \AA^{-1}	2.0 to 2.10 \AA^{-1}

(ii) Order parameter calculations without background subtraction

Shown below are order parameter calculations without implementing a background subtraction. The trends in the order parameter are the same irrespective of whether a background subtraction is implemented.

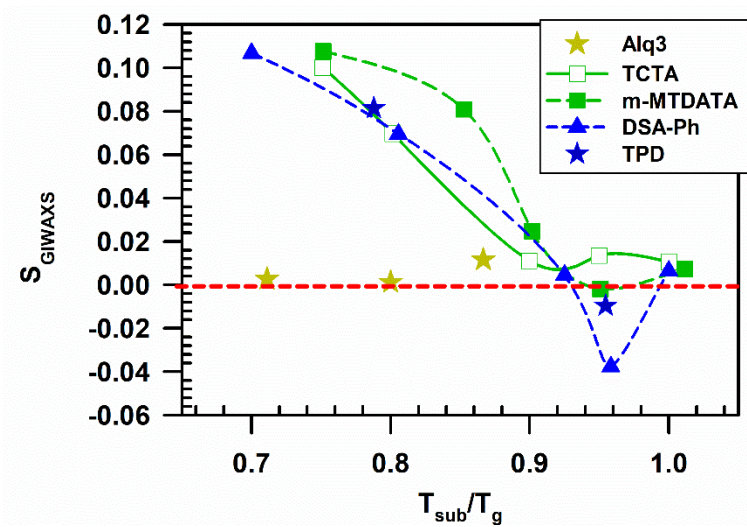


Fig S3: The order parameter calculated as a function of substrate temperature, without an implementation of the background subtraction.