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Supporting information for article:

GIWAXS-SIIRkit: scattering intensity, indexing and refraction calculation toolkit for grazing-incidence wide-angleX-ray scattering of organic materials

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Table S1. Refractive Indices for various materials

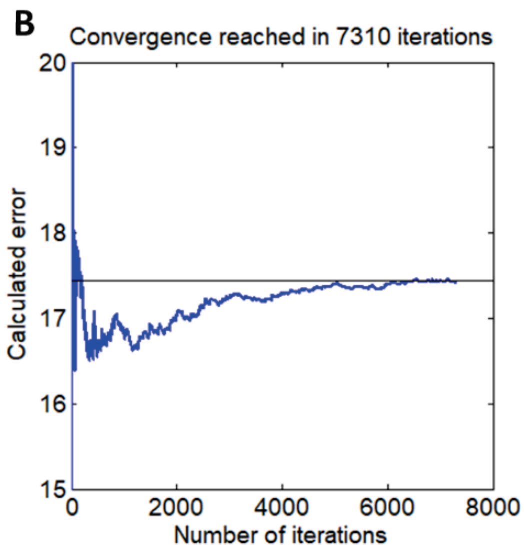
	Name	Chemical Formula	Density (g/cm^3)	Exact β ×10^{-9}	Exact δ ×10^{-6}	Z	A	μ	Approx. δ ×10^{-6}	% error in δ
Polymers	MDMO-PPV	$C_{19}H_{28}O_2$	1.0	0.79	1.41	3.22	5.89	1.0	1.41	0.11%
	P3HT	C_6H_{13}	1.0	0.61	1.48	2.58	4.48	0.8	1.48	0.09%
	P3HT annealed	C_6H_{13}	1.12	0.68	1.65	2.58	4.48	0.9	1.65	0.10%
	PTB7	$C_{41}H_{53}FO_4S_4$	1.12 *	4.29	1.54	3.92	7.35	5.5	1.53	0.31%
	PBDFTPD	$C_{40}H_{53}O_6NS$	1.12	1.90	1.55	3.60	6.69	2.4	1.55	0.17%
	PCDTBT	$C_{43}H_{47}N_3S_3$	1.16	3.63	1.59	3.90	7.31	4.7	1.59	0.25%
	PBDTTPD	$C_{40}H_{53}O_4NS_3$	1.17	3.74	1.62	3.76	7.01	4.8	1.61	0.27%
	PTB7-Th	$C_{49}H_{57}FO_2S_6$	1.20 ¶	5.52	1.64	4.10	7.73	7.1	1.63	0.34%
Small molecules	T1	$C_{64}H_{72}N_4S_8F_2Si$	1.21	5.75	1.64	4.26	8.08	7.4	1.64	0.36%
	DR3TBDTT	$C_{102}H_{128}O_2N_2S_{14}$	1.22 *	6.06	1.68	4.01	7.51	7.8	1.67	0.36%
	X2	$C_{122}H_{148}N_{10}S_{14}Si_3$	1.24	5.71	1.70	4.09	7.70	7.4	1.69	0.35%
Other materials	rubrene	$C_{42}H_{28}$	1.24	0.85	1.67	4.00	7.61	1.1	1.67	0.11%
	ZnPC	$C_{32}H_{16}N_8Zn$	1.49	17.72	1.95	5.16	10.14	22.9	1.94	0.05%
Fullerene derivatives	PC60BM	$C_{72}H_{14}O_2$	1.60	1.21	2.08	5.25	10.35	1.6	2.08	0.13%
	PC71BM	$C_{82}H_{14}O_2$	1.63	1.22	2.12	5.33	10.52	1.6	2.12	0.13%
	C60	C_{60}	1.72 †	1.19	2.12	6.00	12.01	1.5	2.11	0.13%
Substrate materials	Silicon	Si	2.33 ‡	28.27	3.01	14.00	28.09	36.5		
	Silicon dioxide	SiO_2	2.65 ‡	17.83	3.42	10.00	20.03	23.0		
	Microscope slide	72.3% SiO_2; 13.3% Na_2O; 8.8% CaO; 4.3% MgO (by weight)	2.50 §	20.37	3.21	10.26	20.64	26.3		
	Silicon nitride	Si_3N_4	3.17 ‡	24.64	4.09	10	20.04	31.8		
	Indium Tin Oxide (ITO)	90% In_2O_3; 10% SnO_2 (by weight)	7.10 ‖	297.92	7.98	24.14	54.95	384.2		

Table S1. Examples of refractive indices calculated for several materials of interest in OPV calculated at 12.7 keV incident energy, sorted by density. This table also compares the discrepancy between exact δ calculated from first principles and δ calculated using the approximation described in the main text. Densities are taken from Mateker et al. (2015) unless otherwise indicated below. Mateker et al. (2015) measured the densities using X-ray reflectivity. The density of a given film can be affected by processing conditions, so it is important to measure the density of a film fabricated under the same conditions for maximal accuracy.
** approximated from similar materials † taken from Cadek et al. (2010) ‡ taken from Lide (2005) ¶ taken from Mukherjee et al. (2017) § composition and density of a Knittel microscope slide, accessed via Waldemar Knittel Glasbearbeitungs (2019). Using the four most abundant components only. Stoichiometry is* $Si_{1.20}Na_{0.43}Ca_{0.16}Mg_{0.11}O_{2.88}$ *‖ taken from Medvedovski et al. (2008). Stoichiometry is* $In_{6.48}Sn_{0.66}O_{11.05}$

Table S2 Additional figures for scattering intensity calculation

Variable	**Sources of uncertainty**	**Reasonable treatment in most cases**
Incident angle	Calibration inaccuracy; non-planar sample surface	± 0.005 – 0.01°
Sample position (offset)	Uncertainty in sample placement with respect to axis of rotation when aligning by hand	± 3 mm
Beam dimensions, divergence	May not be known very accurately due to measurement difficulty and movement of optical components over time	Does not vary significantly from sample to sample during the course of a single experiment
Beam energy	Usually measured with a high degree of accuracy	Can be assumed to have negligible effect for single crystal monochromators with energy bandwidth of 0.1%; has to be taken into account when multilayer beam pass filters are used with energy bandwidths of about 1%.
Sample dimensions (length, thickness)	Uncertainty in measurement; nonuniformity of film across substrate	± 1 mm length ± 3% thickness, depending on measurement device;larger for nonuniform samples
Sample density	Difficult to measure in a blend film due to multi-phase structure and uncertainty in composition from solvent evaporation or pipetting error; usually approximated based on neat materials	± 0.1 – 0.5 g/cm^3
Sample refractive index	Depends on sample density and composition (see above)	Proportional to density

Table S2. Summary of variables affecting normalization factor calculation



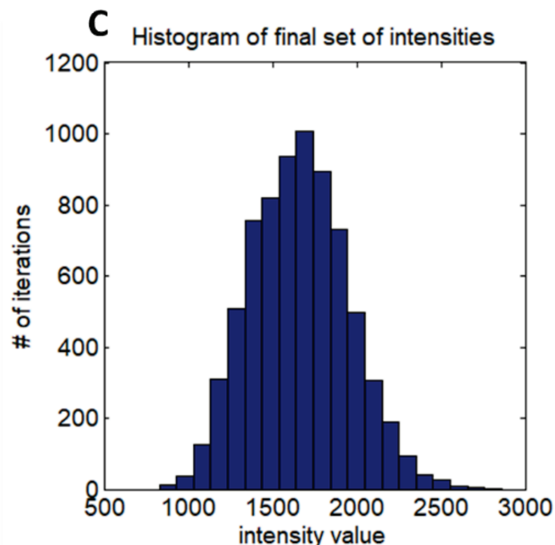


Figure S1. A) GUI setup for simulating uncertainty for a single theoretical PTB7 sample with input parameters described in the text.
B) Convergence in calculated intensity uncertainty for up to 7310 samples generated within the ± parameters. C) Distribution of scattering intensities for final set of generated samples.