Supplementary Information

Understanding Radiation-Generated Electronic Traps in Radiation Dosimeters based on Organic Field-Effect Transistors

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RAD-OFET characterization

Trap density of states (t-DOS) analysis: The t-DOS was calculated using the Grünewald method for the gate-source voltage above the flat band voltage $U_{GS} = |V_{GS} - V_{FB}|$ where V_{FB} was assumed to be the turn-on voltage of the transistor. The interface potential, $V_0(U_{GS})$, is solved for using a root finding method from the equation

$$exp\left(\frac{eV_0}{kT}\right) - \frac{eV_0}{kT} - 1 = \frac{e}{kT}\frac{\varepsilon_i d}{\varepsilon_s l \sigma_0}\left[U_{GS}\sigma(U_{GS}) - \int_0^{U_{GS}} \sigma(\widetilde{U_{GS}})\mathrm{d}\widetilde{U_{GS}}\right]. \quad (1)$$

Where ε_i is the dielectric constant of the dielectric layer, d is the semiconductor thickness, and l is the thickness of the dielectric layer. $\sigma(U_{GS})$ is the field-effect conductivity defined as:

$$\sigma(U_{GS}) = \frac{L}{W}\frac{I_D(U_{GS})}{V_{DS}} \quad (2)$$

where L is the channel length, W is the channel width, V_{DS} is the drain-source voltage, and $I_D(U_{GS})$ is the drain current for particular gate-source voltages, σ_0 is the field-effect conductivity for $U_{GS} = 0$. Using a

derivative method, the solutions of the interface potential can then be used to solve for the carrier density $p(V_0)$ from:

$$p(V_0) = \frac{\varepsilon_0 \varepsilon_i^2}{\varepsilon_s l^2 e} U_{GS} \left(\frac{\mathrm{d}V_0}{\mathrm{d}U_{GS}} \right)^{-1}. \tag{3}$$

The t-DOS can then be obtained via:

$$N(E) \approx \frac{1}{e} \frac{\mathrm{d}p(V_0)}{\mathrm{d}V_0}. \tag{4}$$

A typical method of calculating the derivative steps is using a numerical derivative method such as central finite differences. However, multiple derivatives of noisy data can introduce large numerical errors. Smoothing is typically applied to reduce the effects of the numerical noise, but multiple finite difference derivatives can be sensitive to the type of smoothing applied. Here a forward automatic differentiation method utilizing the ForwardDiff.jl package from the Julia programming language was used to eliminate the numerical noise introduced from the derivatives, with the derivative of the root finding method defined in terms of an adjoint method.

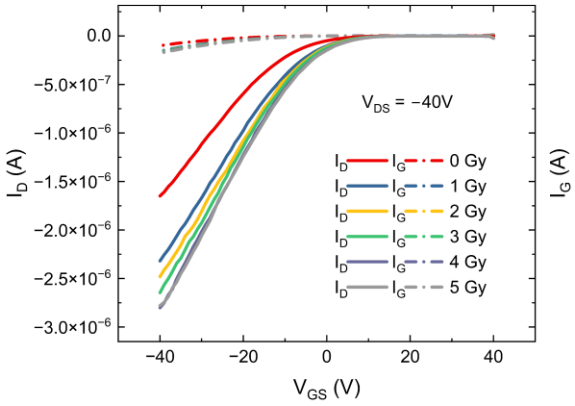

Figure S1 Transfer curves of a transistor exposed to 6 MeV photon radiation. Each curve corresponds to a given dose. The drain current I_D and the gate leakage current I_G are plotted on the same scale for comparison.

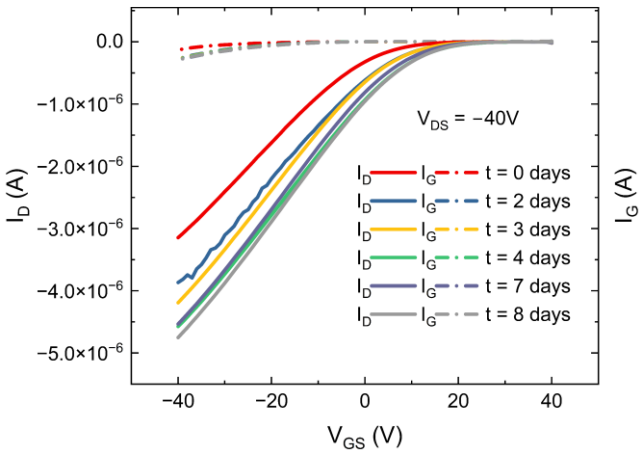

Figure S2 Transfer curves of a reference sample measured at the same time as the transistors exposed to radiation. The drain current I_D and the gate leakage current I_G are plotted on the same scale for comparison.

Error bar calculation: Ten devices of each type have been measured and the values reported in Figures 2a and 2b represent the averages. The error bars in these graphs were calculated using the standard error of the mean and the errors propagated for the average shift in threshold voltage.

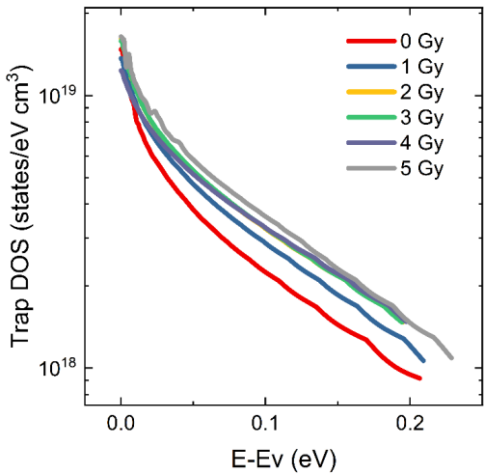

Figure S3 T-DOS of a transistor for varying doses of 6 MeV photon radiation.

Figure S3 presents the t-DOS of a of a transistor for varying doses of 6 MeV photon radiation while Figure S4 presents the t-DOS of a reference sample over the duration of the experiments. Integrating the t-DOS with respect to the energy yields the total trap density given in Table S1. The t-DOS was modelled with a sum of two exponentials using the equation:

$$N(E) = N_1 e^{(-E/E_1)} + N_2 e^{(-E/E_2)} \quad (5)$$

Each term of the sum represents the decay of shallow and deep traps, respectively, as a function of energy. The amplitudes N_1, N_2 and energies E_1, and E_2 are presented in Table S1.

Table S1 The fitting parameters and total trap density for varying radiation doses.

	Fitting Parameters				
Dose (Gy)	**N1 (eV^{-1} cm^{-3})**	**E1 (meV)**	**N2 (eV^{-1} cm^{-3})**	**E2 (meV)**	**Total Trap Density (cm^{-3})**
0	8.6×10^{18}	8.3	6.7×10^{18}	92	6.3×10^{17}
1	6.3×10^{18}	11	7.6×10^{18}	105	7.6×10^{17}
5	7.2×10^{18}	9.9	9.6×10^{18}	103	9.6×10^{17}

Density of interfacial trap states: The density of interfacial trap states, N_{it}^{S}, can be calculated using the equation for the subthreshold slope S

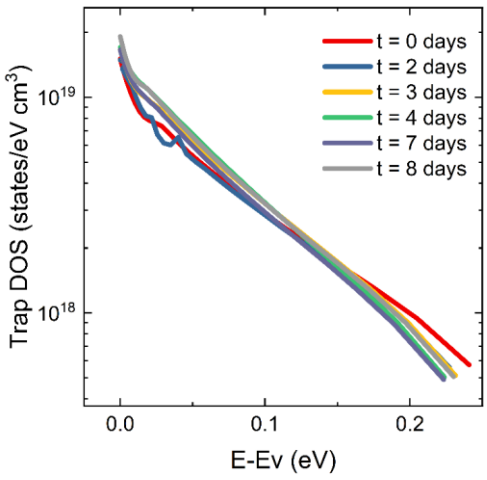

Figure S4 Example of the t-DOS of a reference sample as a function of time. The t-DOS is constant within the accuracy of our analysis.

$$S = \frac{kT\,ln(10)}{e}\left(1 + \frac{e\sqrt{\varepsilon_s N_{bulk}^V} + e^2 N_{it}^S}{C_i}\right) \quad (6)$$

where k is the Boltzmann constant, T is the temperature, e is the elementary charge, ε_s is the semiconductor dielectric constant, C_i is the dielectric capacitance, and N_{bulk}^V is the density of bulk trap states. Setting $N_{bulk}^V = 0$, the upper limit for N_{it}^S can be solved for.

Structural studies fitting protocol

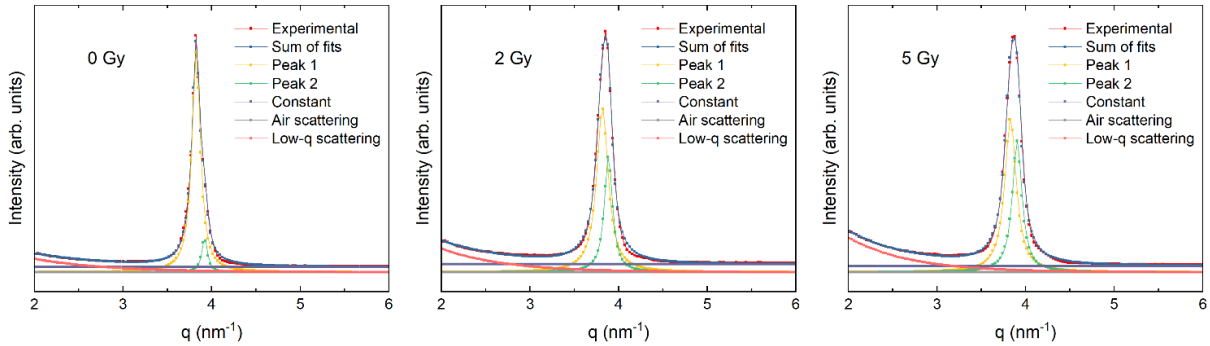

Figure S5 Best fitting results from the main peak, using two Lorentzian peaks, a constant value, the intensity profile from the air scattering pattern and a low-q custom function.

To get the most accurate and comparable fitting results, we applied the same fitting protocol to every diffractogram. The diffractograms were obtained from the 2D patterns after integrating the region of the (001) peak. The integration step was performed using the pyFAI module.[1] Then, without any further data treatment, every intensity profile was fitted to a sum function of two Lorentzian peaks, a constant value, a component from the air scattering (integrated in the same sector of the pattern) and a potential-exponential function, as a low-q scattering component. The complete function is the following:

$$y(q) = Lorentz_1 + Lorentz_2 + A \cdot q^{-4} + B \cdot e^{-k \cdot q} + C + D \cdot air_{scattering} \quad (1)$$

For every diffractogram we used the same restrictions for each parameter and a set of 22,500 combinations of initial parameters. To minimize the computing time, we used a self-made Python script to parallelize the calculations. The following fitting results are the ones with the minimum reduced-χ^2 parameter among the 22,500 starting points for each diffractogram. The parameters for the Lorentzian peaks are compiled in Table S2.

Table S2 Fitting parameters of two Lorentzian peaks.

	Peak 1			**Peak 2**			
Sample	q (nm^{-1})	Sigma (nm^{-1})	Amplitude	q (nm^{-1})	Sigma (nm^{-1})	Amplitude	**A2 / (A1 + A2)**
0 Gy	3.824	0.058	0.533	3.920	0.038	0.055	0.09
2 Gy	3.815	0.079	0.365	3.883	0.056	0.181	0.33
5 Gy	3.827	0.079	0.317	3.902	0.067	0.317	0.50

Notes and references

1 J. Kieffer and D. Karkoulis, *J. Phys.: Conf. Ser.*, 2013, **425**, 202012.