

Electronic supplementary information

Effect of substitution on the charge transport properties of oligophenylenethiolate self-assembled monolayers

Yangbiao Liu,¹ Sonja Katzbach,² Andika Asyuda,¹ Saunak Das,¹
Andreas Terfort,² and Michael Zharnikov^{1,*}

¹ *Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253,
D-69120 Heidelberg, Germany*

² *Institut für Anorganische und Analytische Chemie, Johann Wolfgang Goethe Universität
Frankfurt, Max-von-Laue-Straße 7, D-60438 Frankfurt am Main, Germany*

1. Additional SECO Data: R-PT SAMs

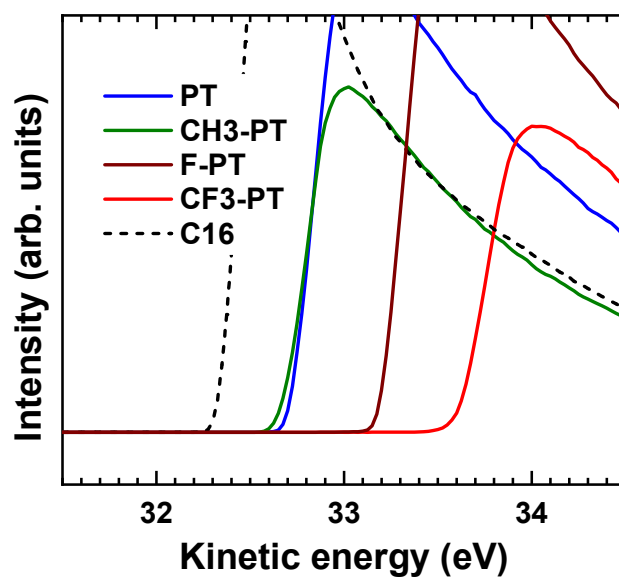


Figure S1. SECO spectra of the R-PT SAMs and the reference C16 monolayer.

2. Charge Transport Data: H-nPT SAMs

Table S1. Overview of the charge transport measurements for the Au/H-nPT//Ga₂O₃/EGaIn junctions.

| SAM | Samples | Junctions | Scans | Processed | Yield |
|------------|----------------|------------------|--------------|------------------|--------------|
| H-PT | 5 | 29 | 381 | 233 | 61.2% |
| H-BPT | 4 | 25 | 283 | 199 | 70.3% |
| H-TPT | 3 | 23 | 317 | 241 | 76.0% |

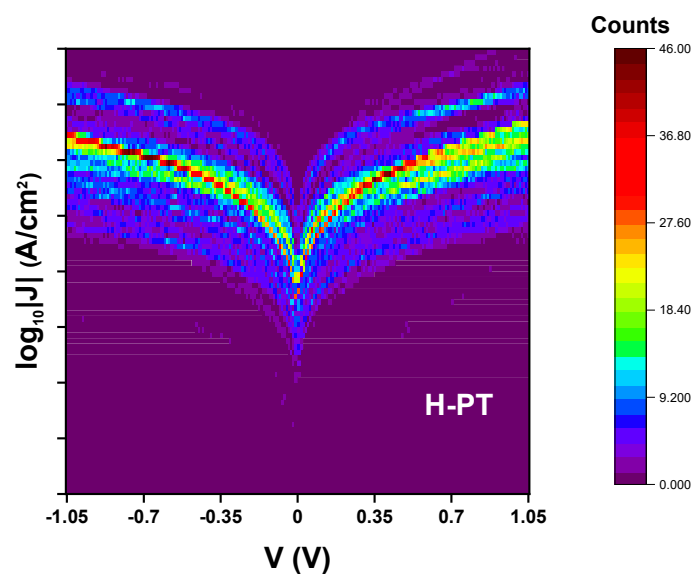


Figure S2. Electrical characteristics of the Au/H-PT//Ga₂O₃/EGaIn junction: Heat map of the semi- $\log_{10} |J(V)|$ curves.

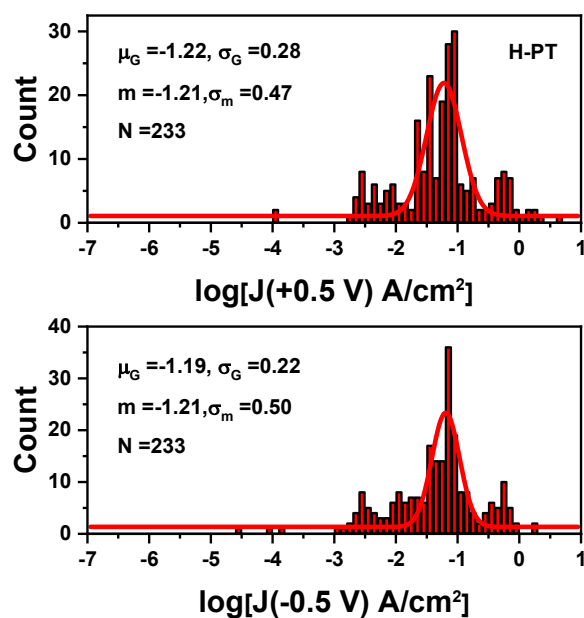


Figure S3. Electrical characteristics of the Au/H-PT//Ga₂O₃/EGaIn junction: Histograms of the $\log_{10} |J|$ at $V = +0.5$ V (top panel) and $V = -0.5$ V (bottom panel). The characteristic parameters are given: μ_G – Gaussian average; σ_G – Gaussian standard deviation; m – median average; σ_m - adjusted median absolute deviation; and N – number of scans.

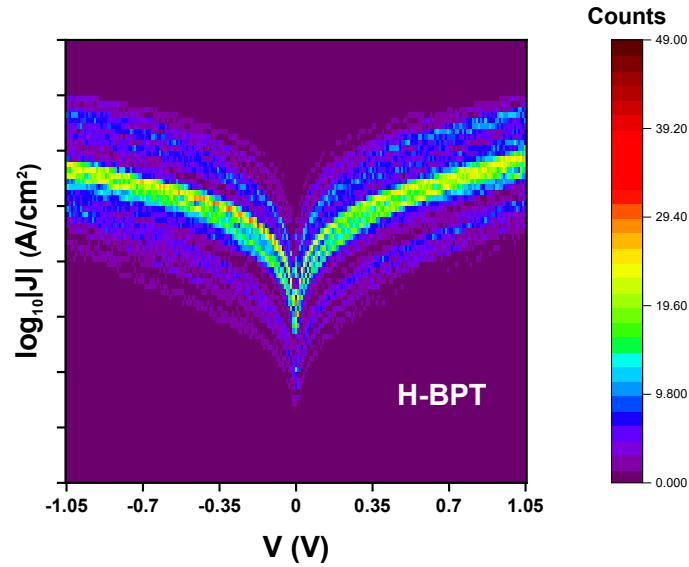


Figure S4. Electrical characteristics of the Au/H-BPT//Ga₂O₃/EGaIn junction: Heat map of the semi- $\log_{10} |J(V)|$ curves.

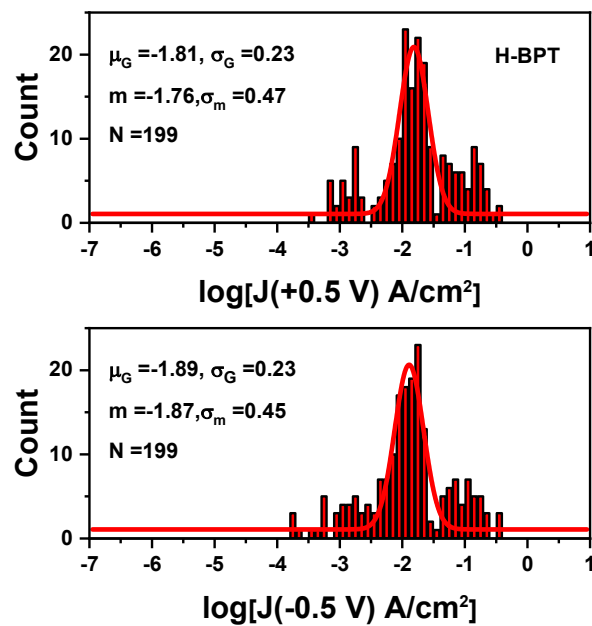


Figure S5. Electrical characteristics of the Au/H-BPT//Ga₂O₃/EGaIn junction: Histograms of the $\log_{10} |J|$ at $V = +0.5$ V (top panel) and $V = -0.5$ V (bottom panel). The characteristic parameters are given: μ_G – Gaussian average; σ_G – Gaussian standard deviation; m – median average; σ_m - adjusted median absolute deviation; and N – number of scans.

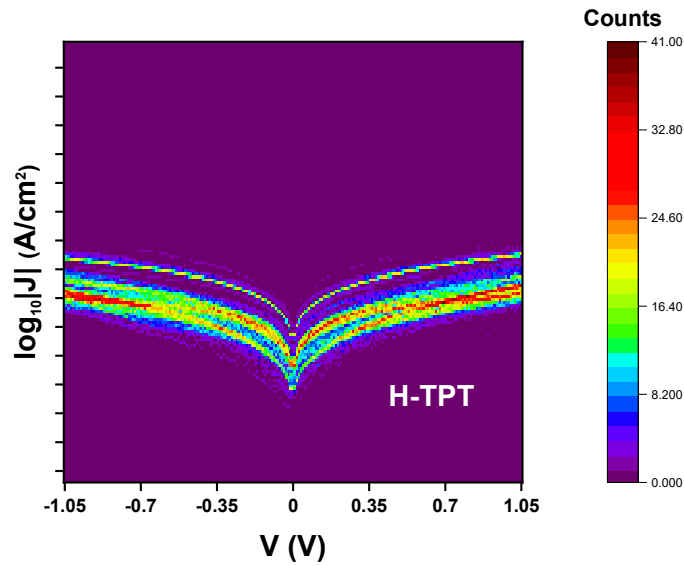


Figure S6. Electrical characteristics of the Au/H-TPT//Ga₂O₃/EGaIn junction: Heat map of the semi- $\log_{10} |J(V)|$ curves.

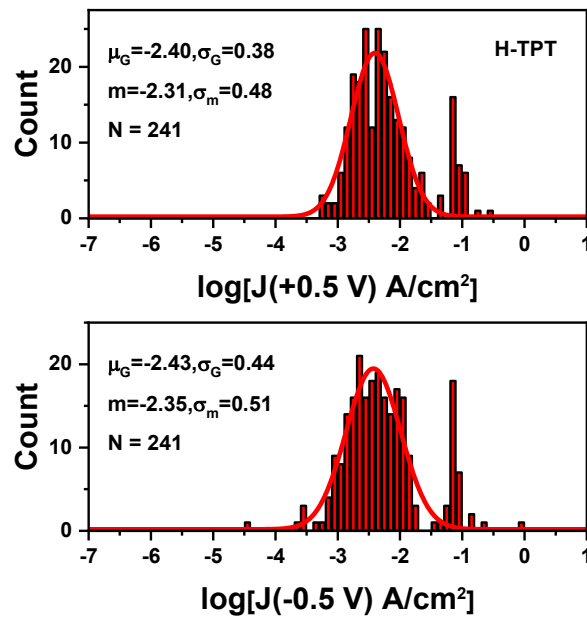


Figure S7. Electrical characteristics of the Au/H-TPT//Ga₂O₃/EGaIn junction: Histograms of the $\log_{10} |J|$ at $V = +0.5$ V (top panel) and $V = -0.5$ V (bottom panel). The characteristic parameters are given: μ_G – Gaussian average; σ_G – Gaussian standard deviation; m – median average; σ_m - adjusted median absolute deviation; and N – number of scans.

3. Charge Transport Data: F-nPT SAMs

Table S2. Overview of the charge transport measurements for the Au/F-nPT//Ga₂O₃/EGaIn junctions.

| SAM | Samples | Junctions | Scans | Processed | Yield |
|------------|----------------|------------------|--------------|------------------|--------------|
| F-PT | 4 | 25 | 430 | 291 | 67.7% |
| F-BPT | 3 | 24 | 232 | 157 | 67.7% |
| F-TPT | 4 | 17 | 243 | 153 | 63.0% |

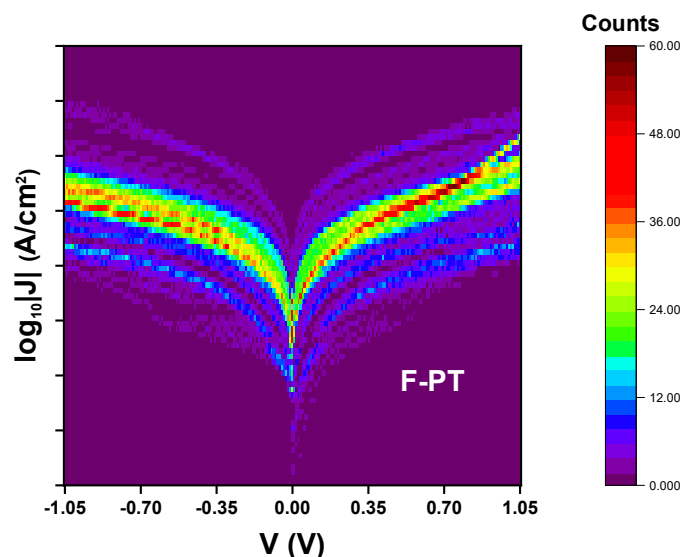


Figure S8. Electrical characteristics of the Au/F-PT//Ga₂O₃/EGaIn junction: Heat map of the semi- $\log_{10}|J(V)|$ curves.

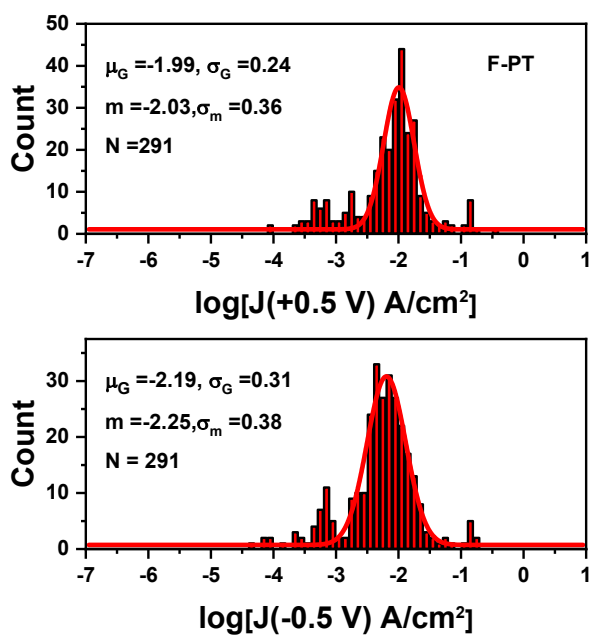


Figure S9. Electrical characteristics of the Au/F-PT//Ga₂O₃/EGaIn junction: Histograms of the $\log_{10}|J|$ at $V = +0.5$ V (top panel) and $V = -0.5$ V (bottom panel). The characteristic parameters are given: μ_G – Gaussian average; σ_G – Gaussian standard deviation; m – median average; σ_m - adjusted median absolute deviation; and N – number of scans.

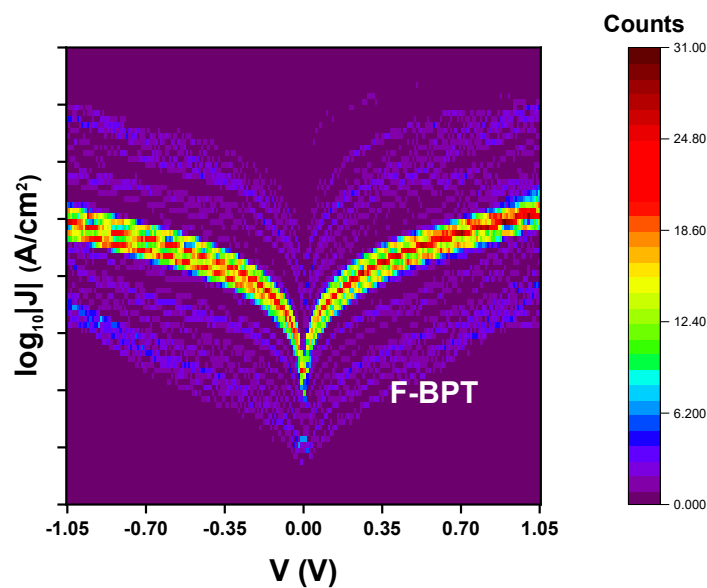


Figure S10. Electrical characteristics of the Au/F-BPT//Ga₂O₃/EGaIn junction: Heat map of the semi-log₁₀ |J(V)| curves.

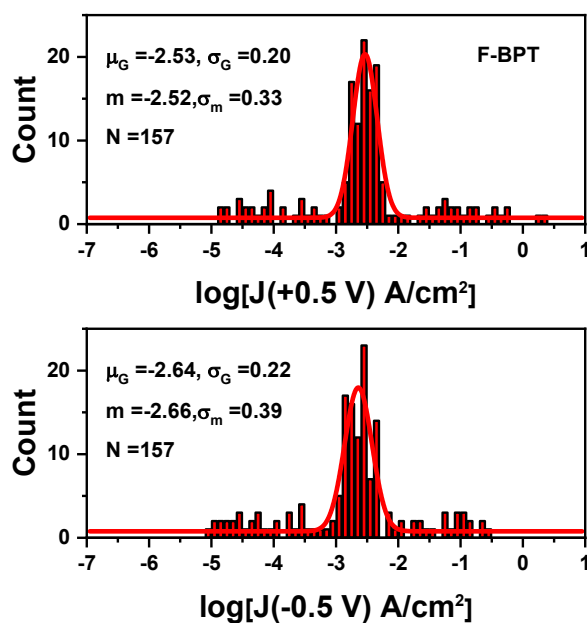


Figure S11. Electrical characteristics of the Au/F-BPT//Ga₂O₃/EGaIn junction: Histograms of the log₁₀ |J| at V = +0.5 V (top panel) and V = -0.5 V (bottom panel). The characteristic parameters are given: μ_G – Gaussian average; σ_G – Gaussian standard deviation; m – median average; σ_m - adjusted median absolute deviation; and N – number of scans.

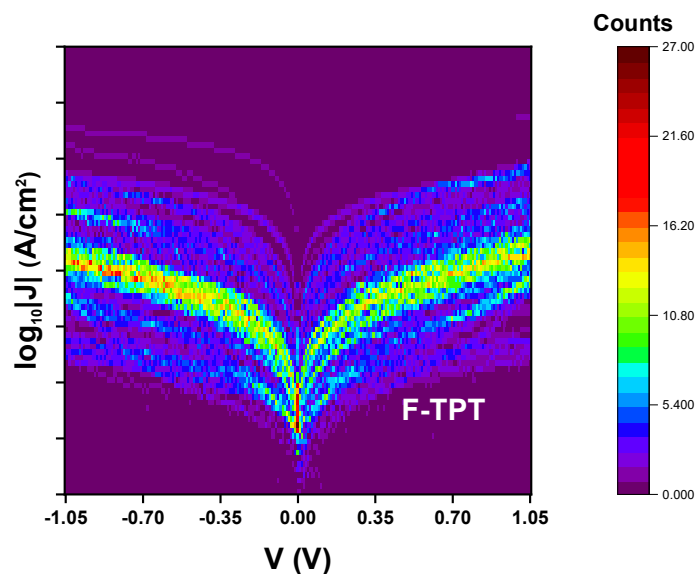


Figure S12. Electrical characteristics of the Au/F-TPT//Ga₂O₃/EGaIn junction: Heat map of the semi- $\log_{10} |J(V)|$ curves.

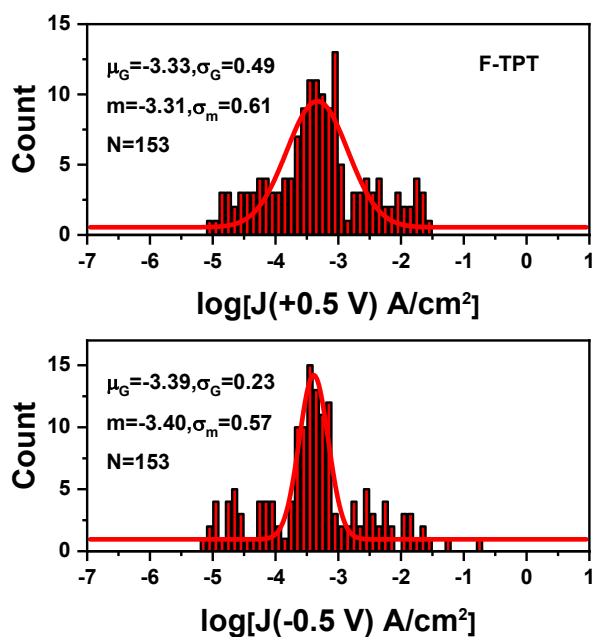


Figure S13. Electrical characteristics of the Au/F-TPT//Ga₂O₃/EGaIn junction: Histograms of the $\log_{10} |J|$ at $V = +0.5$ V (top panel) and $V = -0.5$ V (bottom panel). The characteristic parameters are given: μ_G – Gaussian average; σ_G – Gaussian standard deviation; m – median average; σ_m – adjusted median absolute deviation; and N – number of scans.

4. Charge Transport Data: CH₃-nPT SAMs

Table S3. Overview of the charge transport measurements for the Au/CH₃-nPT//Ga₂O₃/EGaIn junctions.

| SAM | Samples | Junctions | Scans | Processed | Yield |
|----------------------|----------------|------------------|--------------|------------------|--------------|
| CH ₃ -PT | 3 | 30 | 254 | 160 | 63.0% |
| CH ₃ -BPT | 2 | 16 | 241 | 146 | 60.6% |
| CH ₃ -TPT | 3 | 17 | 292 | 184 | 63.0% |

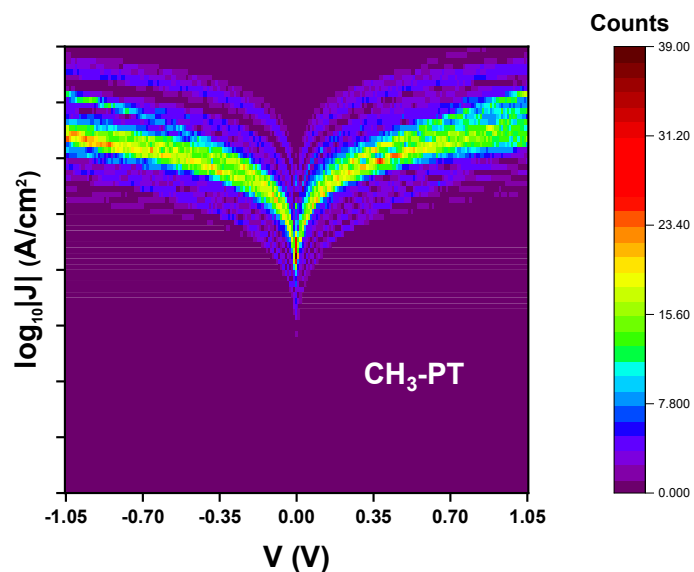


Figure S14. Electrical characteristics of the Au/CH₃-PT//Ga₂O₃/EGaIn junction: Heat map of the semi-log₁₀ |J(V)| curves.

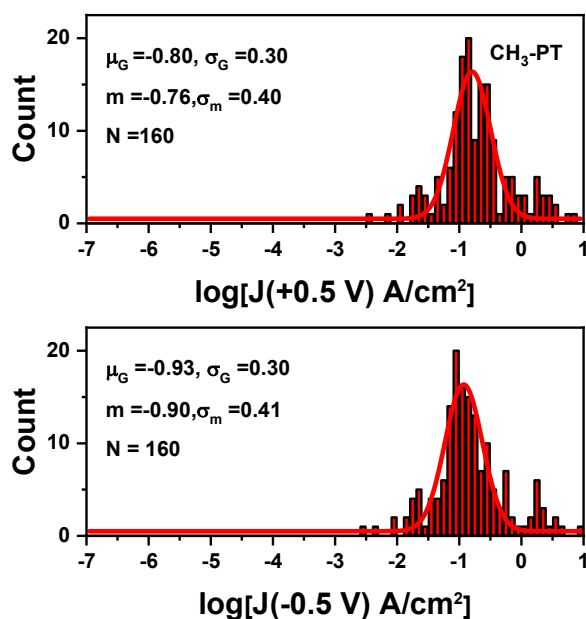


Figure S15. Electrical characteristics of the Au/CH₃-PT//Ga₂O₃/EGaIn junction: Histograms of the log₁₀ |J| at V = +0.5 V (top panel) and V = -0.5 V (bottom panel). The characteristic parameters are given: μ_G – Gaussian average; σ_G – Gaussian standard deviation; m – median average; σ_m - adjusted median absolute deviation; and N – number of scans.

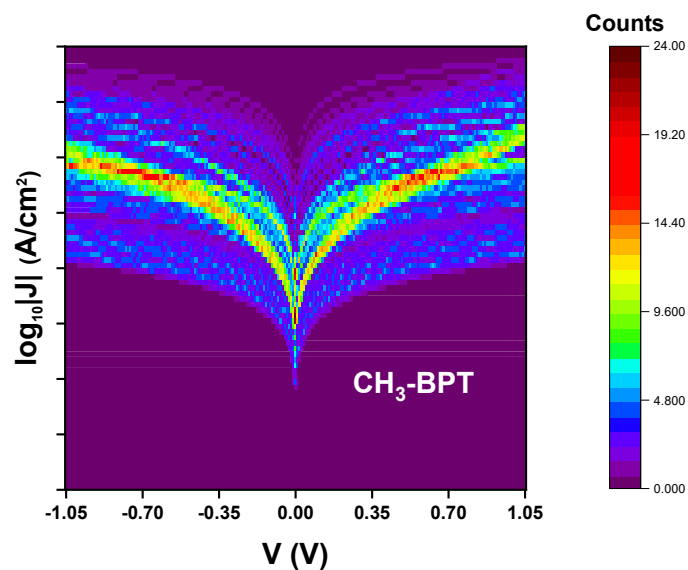


Figure S16. Electrical characteristics of the Au/CH₃-BPT//Ga₂O₃/EGaIn junction: Heat map of the semi- $\log_{10} |J(V)|$ curves.

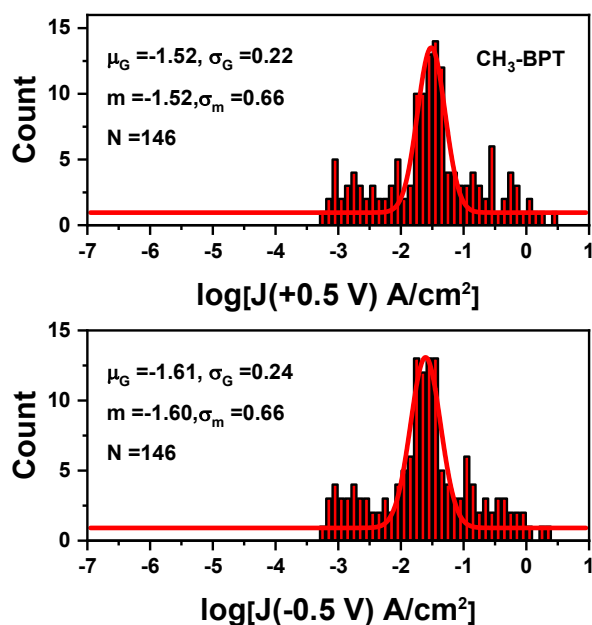


Figure S17. Electrical characteristics of the Au/CH₃-BPT//Ga₂O₃/EGaIn junction: Histograms of the $\log_{10} |J|$ at $V = +0.5$ V (top panel) and $V = -0.5$ V (bottom panel). The characteristic parameters are given: μ_G – Gaussian average; σ_G – Gaussian standard deviation; m – median average; σ_m – adjusted median absolute deviation; and N – number of scans.

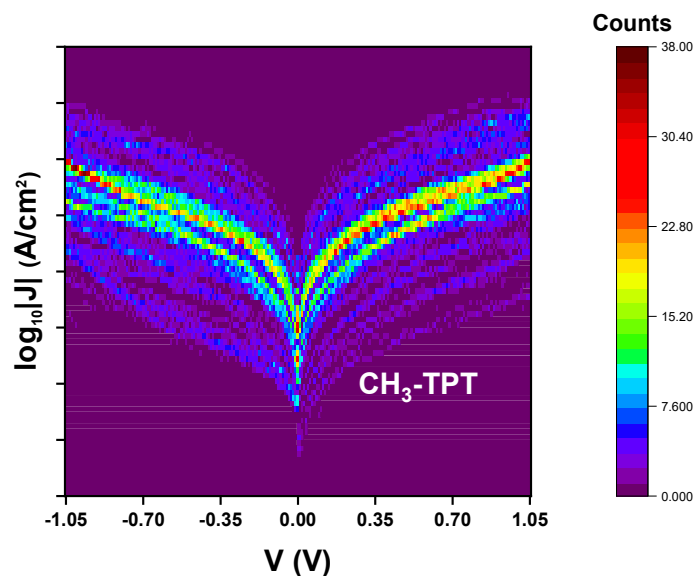


Figure S18. Electrical characteristics of the Au/CH₃-TPT//Ga₂O₃/EGaIn junction: Heat map of the semi- $\log_{10} |J(V)|$ curves.

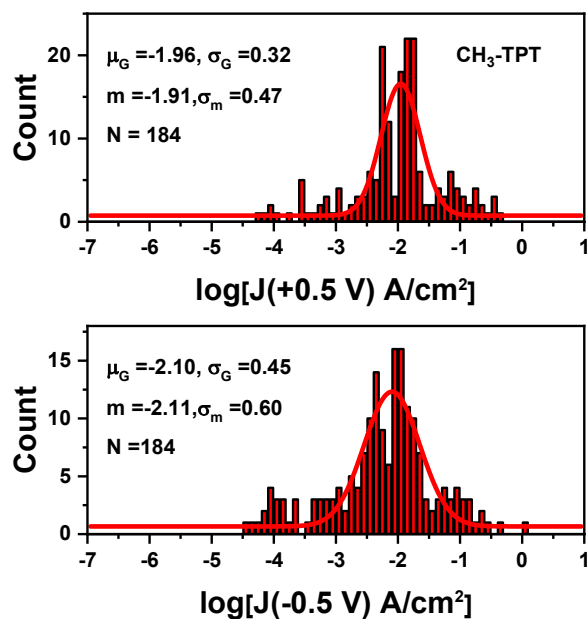


Figure S19. Electrical characteristics of the Au/CH₃-TPT//Ga₂O₃/EGaIn junction: Histograms of the $\log_{10} |J|$ at $V = +0.5$ V (top panel) and $V = -0.5$ V (bottom panel). The characteristic parameters are given: μ_G – Gaussian average; σ_G – Gaussian standard deviation; m – median average; σ_m - adjusted median absolute deviation; and N – number of scans.

5. Charge Transport Data: CF₃-nPT SAMs

Table S4. Overview of the charge transport measurements for the Au/CF₃-nPT//Ga₂O₃/EGaIn junctions.

| SAM | Samples | Junctions | Scans | Processed | Yield |
|------------|----------------|------------------|--------------|------------------|--------------|
| CF3-PT | 3 | 18 | 244 | 179 | 73.4% |
| CF3-BPT | 2 | 21 | 232 | 161 | 69.4% |
| CF3-TPT | 3 | 30 | 272 | 181 | 66.5% |

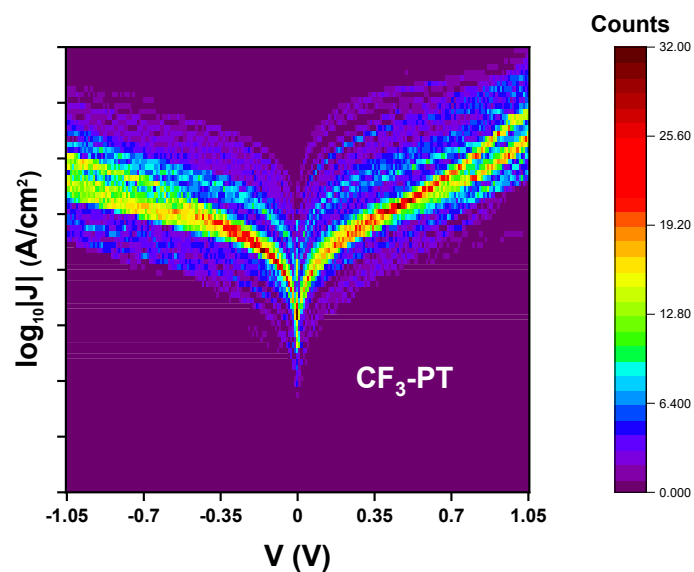


Figure S20. Electrical characteristics of the Au/CF₃-PT//Ga₂O₃/EGaIn junction: Heat map of the semi-log₁₀ |J(V)| curves.

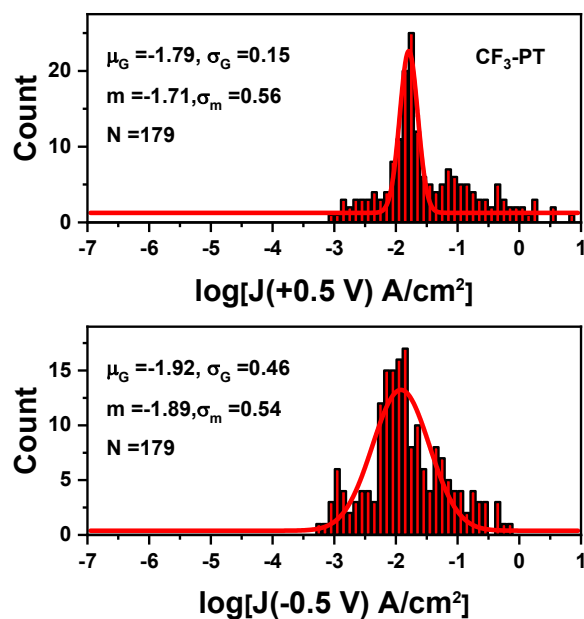


Figure S21. Electrical characteristics of the Au/CF₃-PT//Ga₂O₃/EGaIn junction: Histograms of the log₁₀ |J| at V = +0.5 V (top panel) and V = -0.5 V (bottom panel). The characteristic parameters are given: μ_G – Gaussian average; σ_G – Gaussian standard deviation; m – median average; σ_m – adjusted median absolute deviation; and N – number of scans.

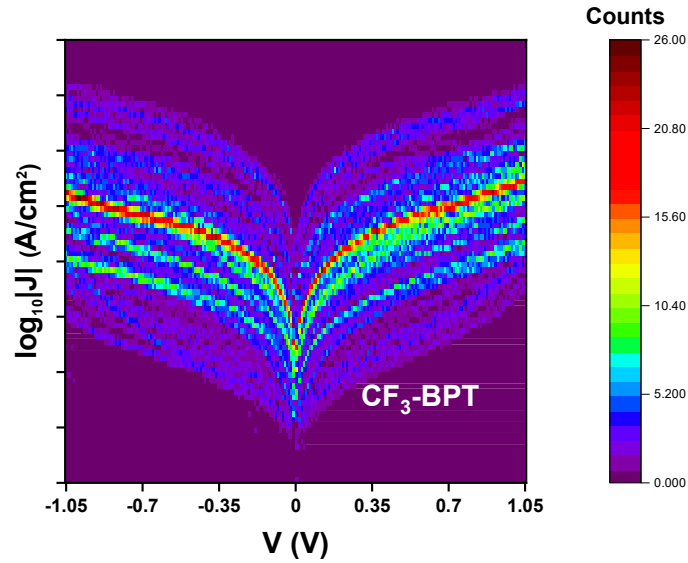


Figure S22. Electrical characteristics of the Au/CF₃-BPT//Ga₂O₃/EGaIn junction: Heat map of the semi-log $|J(V)|$ curves.

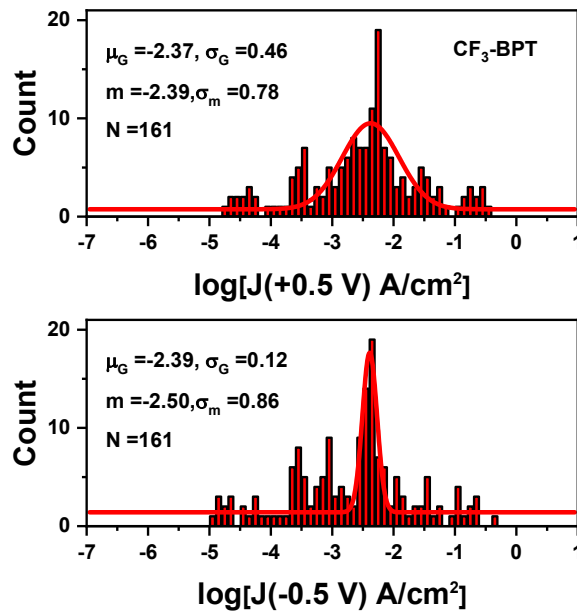


Figure S23. Electrical characteristics of the Au/CF₃-BPT//Ga₂O₃/EGaIn junction: Histograms of the $\log_{10}|J|$ at $V = +0.5$ V (top panel) and $V = -0.5$ V (bottom panel). The characteristic parameters are given: μ_G – Gaussian average; σ_G – Gaussian standard deviation; m – median average; σ_m - adjusted median absolute deviation; and N – number of scans.

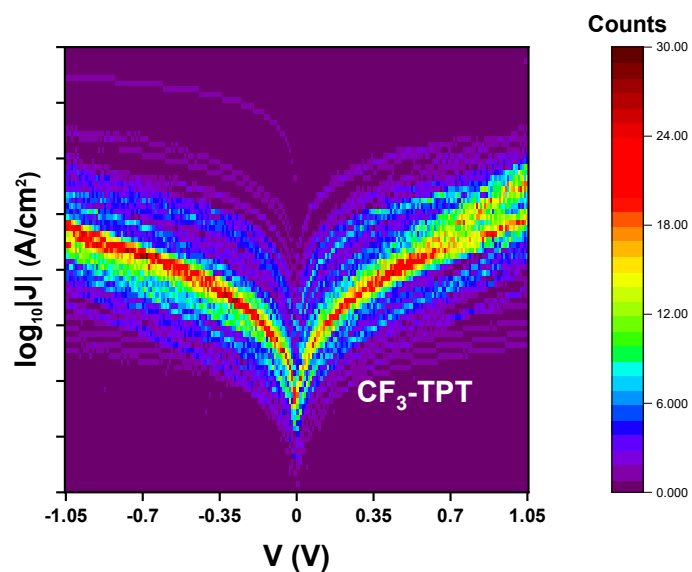


Figure S24. Electrical characteristics of the Au/CF₃-TPT//Ga₂O₃/EGaIn junction: Heat map of the semi-log₁₀ |J(V)| curves.

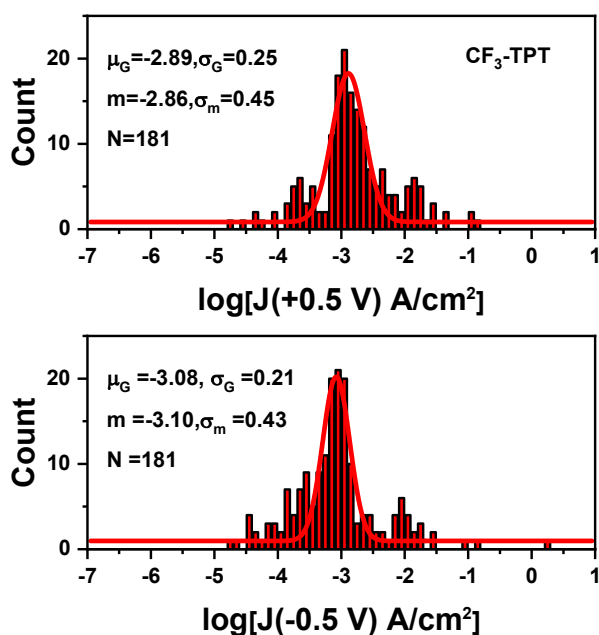


Figure S25. Electrical characteristics of the Au/CF₃-TPT//Ga₂O₃/EGaIn junction: Histograms of the log₁₀ |J| at V = +0.5 V (top panel) and V = -0.5 V (bottom panel). The characteristic parameters are given: μ_G – Gaussian average; σ_G – Gaussian standard deviation; m – median average; σ_m - adjusted median absolute deviation; and N – number of scans.

6. Rectification Ratio

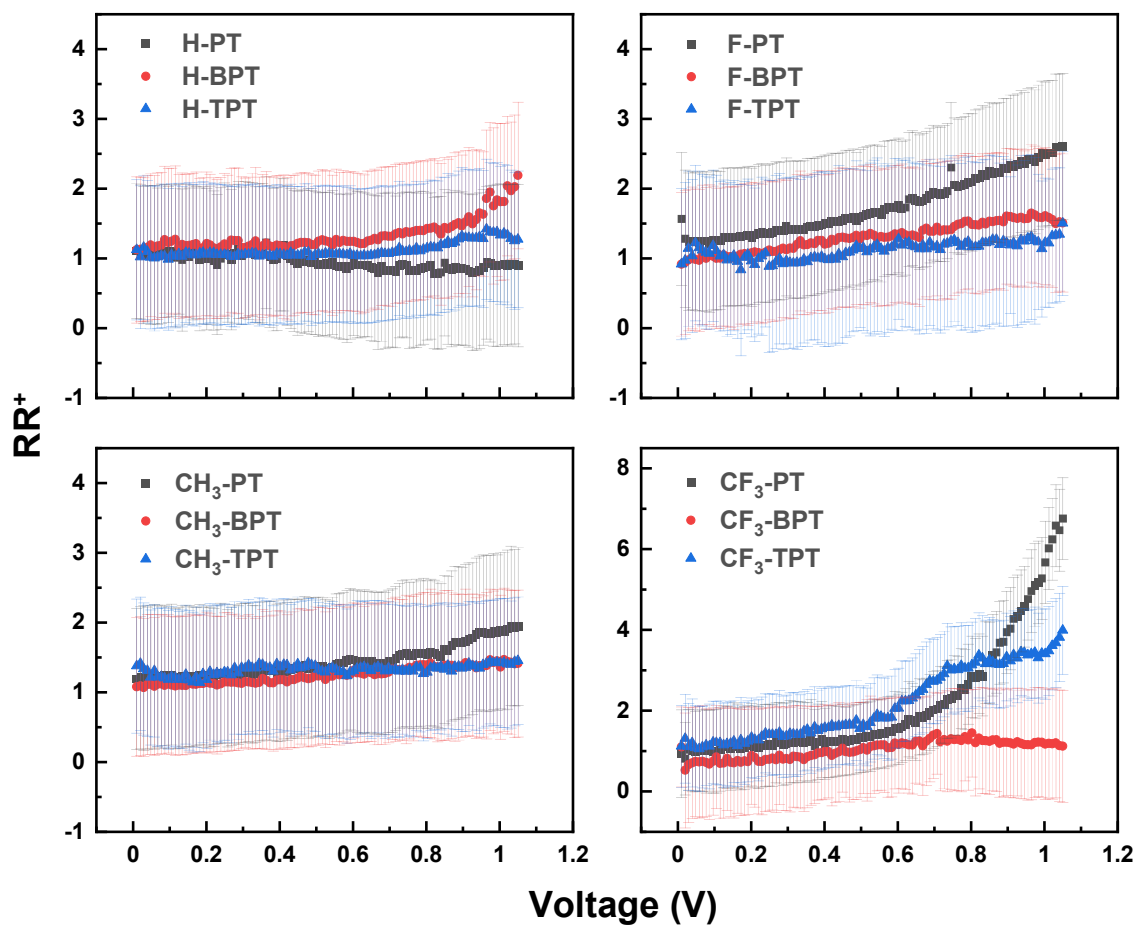


Figure S26. Rectification ratio of the R-nPT SAMs measured in the Au/SAM//Ga₂O₃/EGaIn junctions. The higher current density was observed at the positive bias voltages.