ADVANCED MATERIALS INTERFACES

# Supporting Information

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## Influence of the Surface Treatment on the Solution Coating of Single-Crystalline Organic Thin-Films

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# Influence of the surface treatment on the solution coating of highly crystalline organic thin-films

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## SUPPORTING INFORMATION



| Solvent | Temperature | Coating speed |
|---|---|---|
| Heptane | 20°C | 25 µm/s |
| Heptane | 50°C | 91 µm/s |
| Toluene | 20°C | 11 µm/s |
| Toluene | 50°C | 43 µm/s |
| Chlorobenzene | 50°C | 21 µm/s |

**Table S1:** Coating speeds used in this study. Speed were determined according to our previously reported model[1].

| Surface treatment | Water | Ethylene glycol | Chloro-benzene | Diiodo-methane |
|---|---|---|---|---|
| SiO2 | <5° | - | <5° | 39° |
| HMDS | 65° | 40° | 23° | 54° |
| APTS | 68° | 44° | <5° | 43° |
| PETS | 82° | 50° | <5° | 42° |
| ODTS | 109° | 82° | 39° | 66° |
| DDTS | 109° | 83° | 42° | 68° |
| FDTS | 111° | 100° | 75° | 100° |
| PFBT | 72° | 40° | <5° | 38° |
| PETMS | 84° | 52° | <5° | 40° |
| ODTMS | 109° | 76° | 38° | 65° |
| DDTMS | 106° | 75° | 36° | 64° |

**Table S2:** Overview over the measured contact angles used for the calculation of the surface energy and its individual dispersive and polar components.

| Solvent | $\sigma$ | $\sigma_{disp}$ | $\sigma_{polar}$ | Reference |
|---|---|---|---|---|
| Hexane | 17.4 | 17.4 | 0.0 | Panzer[2] |
| Heptane* | 20.4 | 20.4 | 0.0 | Fowkes[3] |
| Methanol | 22.1 | 12.4 | 9.7 | Panzer[2] |
| Ethanol | 22.2 | 15.8 | 6.4 | Panzer[2] |
| Acetone | 23.3 | 16.5 | 6.8 | Panzer[2] |
| Dichloromethane (DCM) | 26.5 | 23.2 | 3.3 | Janczuk[4] |
| Chloroform | 27.1 | 24.8 | 2.3 | Janczuk[4] |
| Tetrahydrofuran | 27.7 | 22.8 | 4.9 | Panzer[2] |
| Toluene* | 28.5 | 27.2 | 1.3 | Janczuk[4] |
| Mesitylene | 28.8 | 27.9 | 0.9 | Janczuk[4] |
| m-Xylene | 28.9 | 27.9 | 1.0 | Janczuk[4] |
| Chlorobenzene*,† | 33.6 | 32.4 | 1.2 | Janczuk[4] |
| Anisole | 34.6 | 30.7 | 3.9 | Panzer[2] |
| Dimethyl formamide (DMF) | 36.5 | 25.2 | 11.3 | Ghorai[5] |
| Dimethyl sulfoxide (DMSO) | 43.0 | 25.4 | 17.6 | Panzer[2] |
| Aniline | 43.1 | 33.9 | 9.2 | Panzer[2] |
| Ethylene glycol† | 48.2 | 18.9 | 29.3 | Janczuk[6] |
| Diiodomethane† | 50.8 | 48.5 | 2.3 | Fowkes[3] |
| Water† | 72.8 | 21.8 | 51.0 | Fowkes[3] |

**Table S3:** Literature surface tension ($\sigma$) data with their dispersive ($\sigma_{disp}$) and polar ($\sigma_{polar}$) component for several common liquids (in mN/m). *Liquids used for zone casting experiments. †Liquids used for surface energy calculations of different surface treatments.

| Solvent | SiO2 | HMDS | APTS | PETS | ODTS | DDST | FDTS | PFBT | PETMS | ODTMS | DDTMS |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Hexane | - | - | - | - | - | - | 54° | - | - | - | - |
| Heptane | - | - | - | - | - | - | 60° | - | - | - | - |
| Methanol | - | - | - | - | 40° | 39° | 49 | - | - | 31° | 22° |
| Ethanol | - | - | - | - | 6° | 7° | 45° | - | - | 3° | - |
| Acetone | - | - | - | - | 18° | 19° | 49° | - | - | 10° | 5° |
| DCM | - | - | - | - | 8° | 11° | 61 | - | - | 6° | - |
| Chloroform | - | - | - | - | 9° | 13° | 65° | - | - | 6° | - |
| Tetrahydrofuran | - | - | - | - | 23° | 26° | 62° | - | - | 13° | 12° |
| Toluene | - | - | - | - | 17° | 23° | 72° | - | - | 14° | 9° |
| Mesitylene | - | - | - | - | 21° | 26° | 74° | - | - | 19° | 16° |
| m-xylene | - | - | - | - | 21° | 26° | 74° | - | - | 19° | 16° |
| Chlorobenzene | - | 20° | - | - | 38° | 41° | 81° | - | - | 37° | 35° |
| Anisole | - | - | - | - | 42° | 44° | 76° | - | - | 38° | 24° |
| DMF | - | - | - | - | 57° | 58° | 76° | - | - | 53° | 49° |
| DMSO | - | - | - | 24° | 71° | 72° | 85° | - | 27° | 68° | 65° |
| Aniline | - | 6° | - | 5° | 61° | 62° | 84° | - | 8° | 58° | 55° |

**Table S4:** Calculated contact angles for some of the most commonly used organic solvents on varying self-assembled monolayers. We used the theory of Wu[7,8] to calculate the contact angles based on the surface energy values from Table S3.

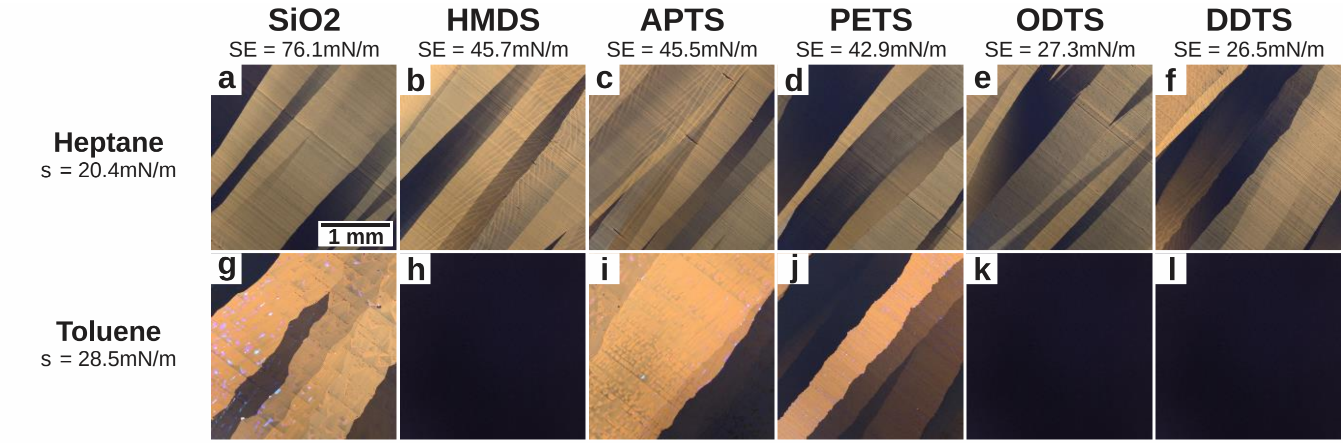


**Figure S1.** Coating at elevated temperatures of 50°C for $C_8$-BTBT solutions of (a-f) heptane and (g-l) toluene. No obvious difference for fully covered films between different surface treatments is visible. There was no coverage on top of FDTS treated substrates. For better visibility, it was not included here.

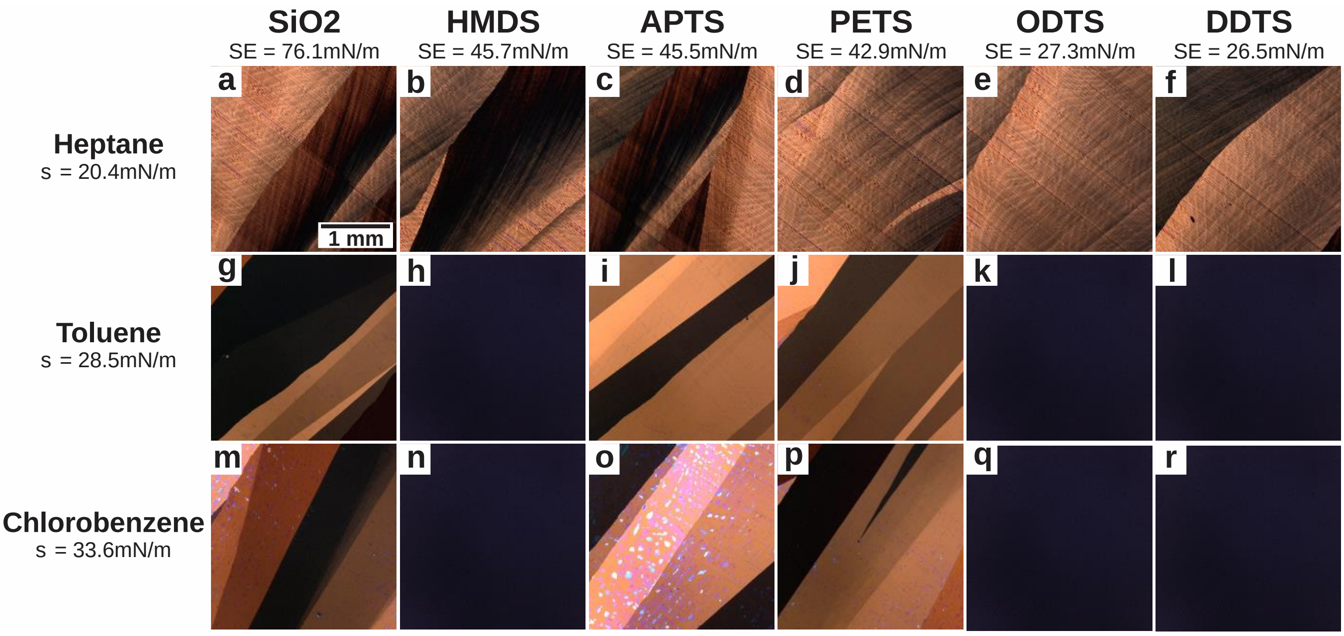


**Figure S2.** Coating with TIPS-Pentacene. Heptane was coated at room temperature, toluene and chlorobenzene at 50°C. No obvious difference for fully covered films between different surface treatments is visible. There was no coverage on top of FDTS treated substrates. For better visibility, it was not included here.

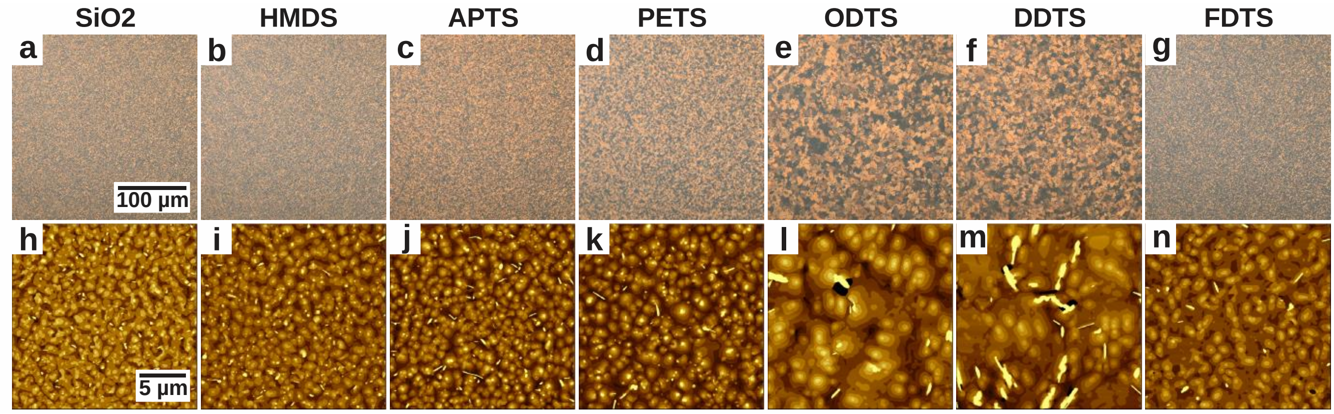


**Figure S3.** Morphology of evaporated C8-BTBT films for different substrate treatments. (a-g) polarized light microscopy images, (h-n) AFM images of these films.

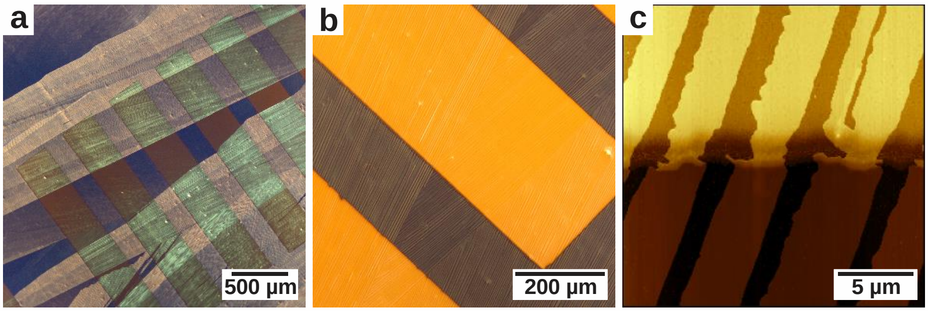


**Figure S4.** Coating over 100 nm thick Au bottom contact pads. No obvious influence on the long- and short-range morphology is visible.

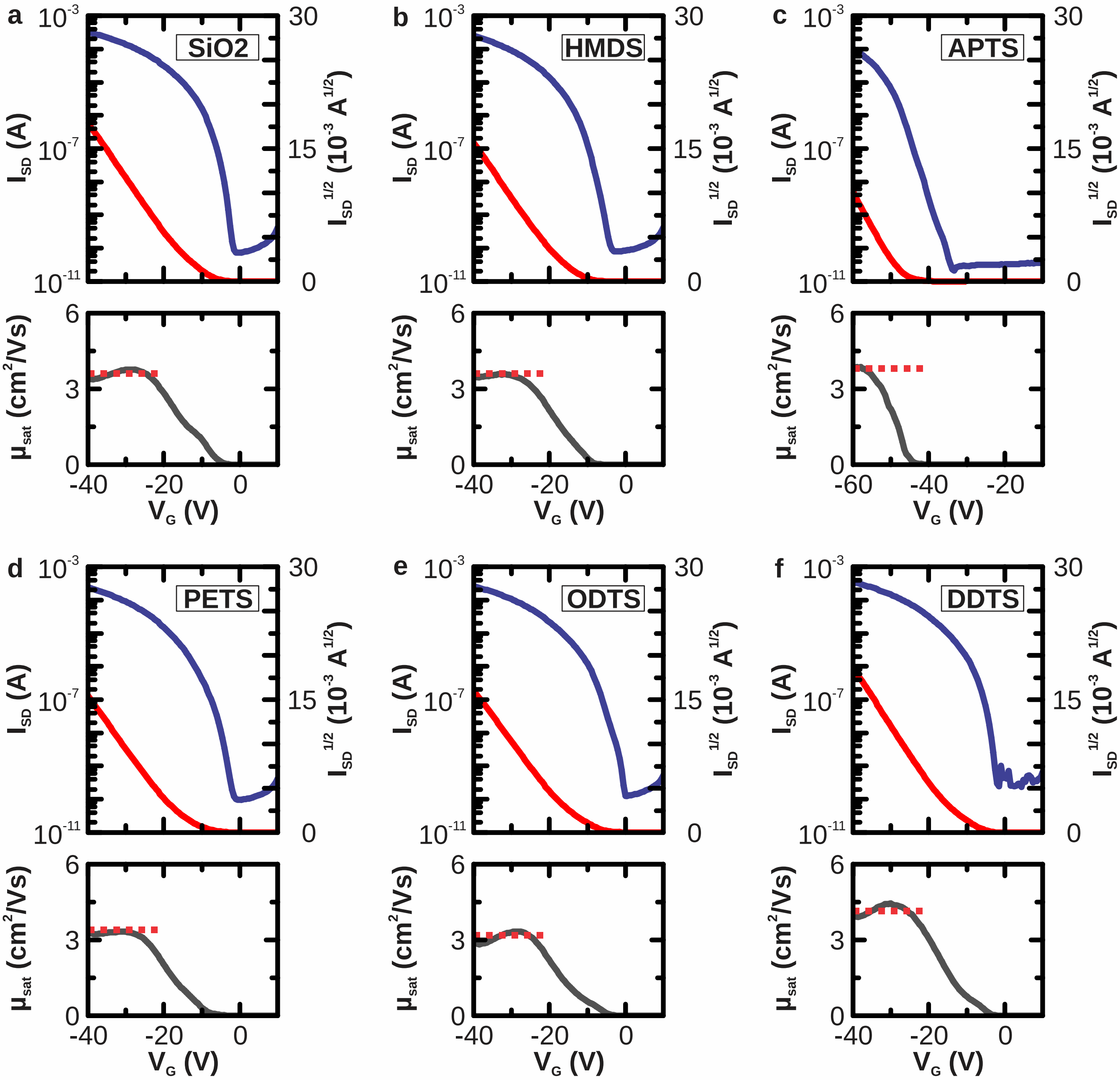


**Figure S5.** Typical electrical characteristics of zone-cast samples on different surface treatments. Transfer and mobility curves of bottom-gate, top-contact type OTFT. Leakage currents stayed below $10^{-9}$ A for all measured devices independent of $V_G$. Red dotted line in the mobility plot shows the mobility average mobility of the 200 OTFTs. As the APTS treatment yields deep onset and threshold voltages in (c), the measurement range for this sample is extended to VG = -60 V to reveal the start of mobility saturation.

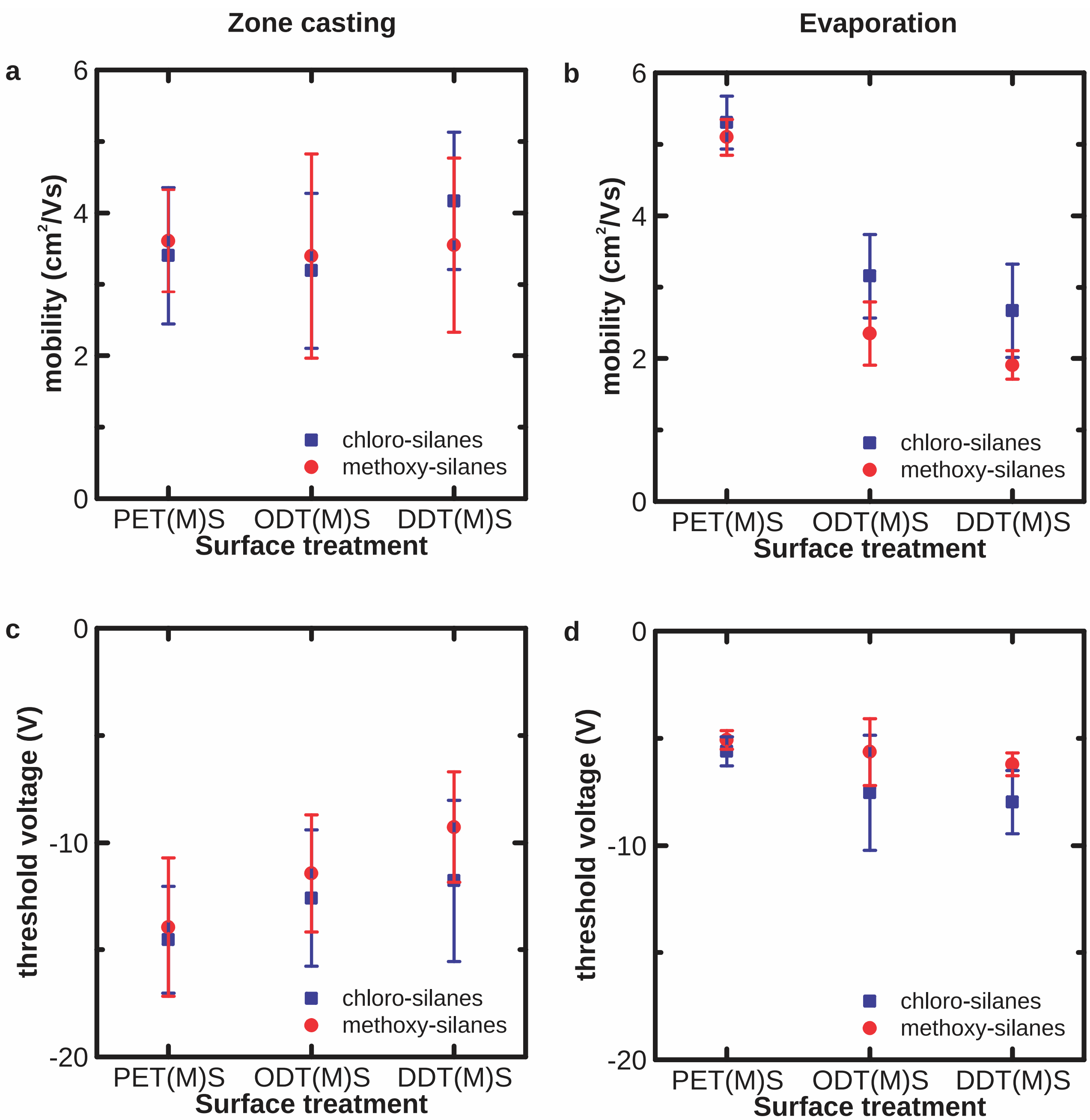


**Figure S6.** Comparison of electrical results of zone cast and evaporated films on methoxy- and chloro-terminated silanes with the same core. (a) Extracted saturation mobility for zone cast films and (b) for evaporated films. (c) Threshold voltages for the zone cast films and (d) for evaporated films. Both types of treatments deliver similar surface energies, despite differences in aerial density (Table 2). For the zone cast samples, the average aggregate mobility is again independent from the surface treatment and the average threshold voltages for the methoxy-terminated silane treatments are slightly closer to 0 V (b). In the case of evaporation, we notice a similar trend in the threshold voltages (c) and the mobilities are all slightly smaller for the methoxy-terminated silanes treatments (d). We speculate that this last effect is related to the lower aerial density of the methoxy-terminated silane treatments that negatively impact film morphology.

## Supplementary References


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