

Supporting Information

Driving forces for the self-assembly of graphene oxide on organic monolayers

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I. Methods

1. The calculation of the dipole moment

The dipole moments and geometries are all calculated by DFT calculations in the Gaussian 09 program¹, using the PBE functional² and the SVP/SVPfit basis set^{3,4}. All dipole moments are given in the chemical (IUPAC) form, which means that they point from negative to positive charge density, and the unit is Debye. All dipole moments represent the projection of the molecular dipole moment along the axis defined by the phosphorous atom of the anchor group and the C₁₀ atom of the alkyl chain, which means that the axis is perpendicular to and goes out of the surface.

The dipole moments have been calculated for different possible rotational conformers (rotamers) of the anchor group (the phosphonic acid group) and functional headgroups (e.g. the hydroxyl group). The value presented in Table 1 is the dipole moment for the rotamer which is lowest in energy (most stable), Boltzmann weighted by their relative energy.

2. SAM Formation Parameters

Table S1: SAM formation parameters

	Concentration (mM)	Immersion Time (hours)
HO-C ₁₁ -PA	0.2	~24
HS-C ₁₂ -PA	0.2	~24
MIM ⁺ -C ₁₂ -PA	0.025	4
NH ₃ ⁺ -C ₁₂ -PA	0.05	1
HOOC-C ₁₅ -PA	0.2	~24

II. Figures

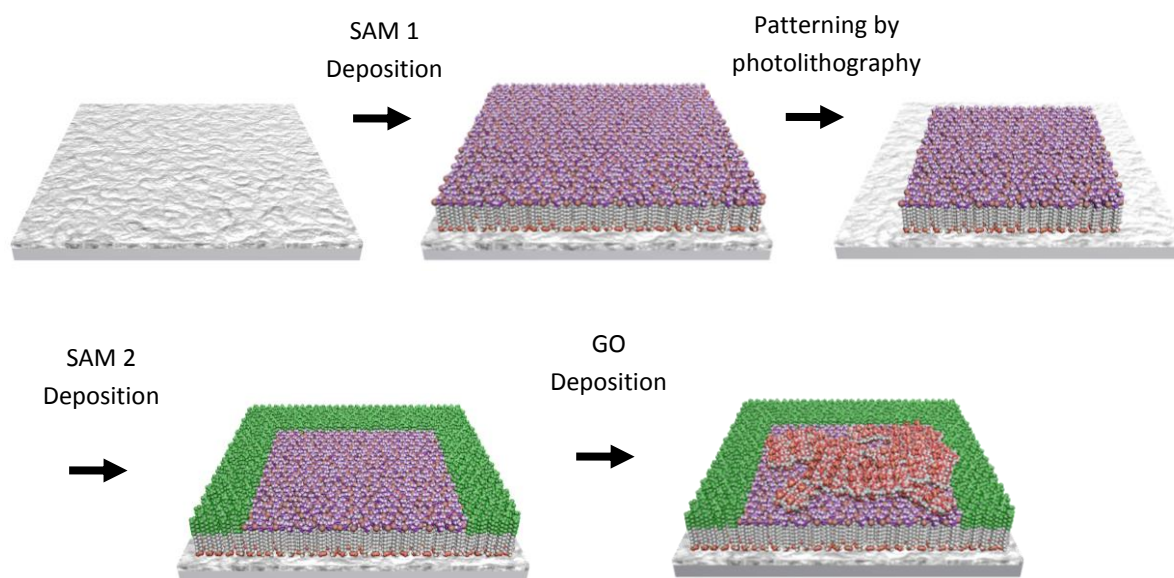


Figure S1. Schematic fabrication process of in-plane patterned substrates.

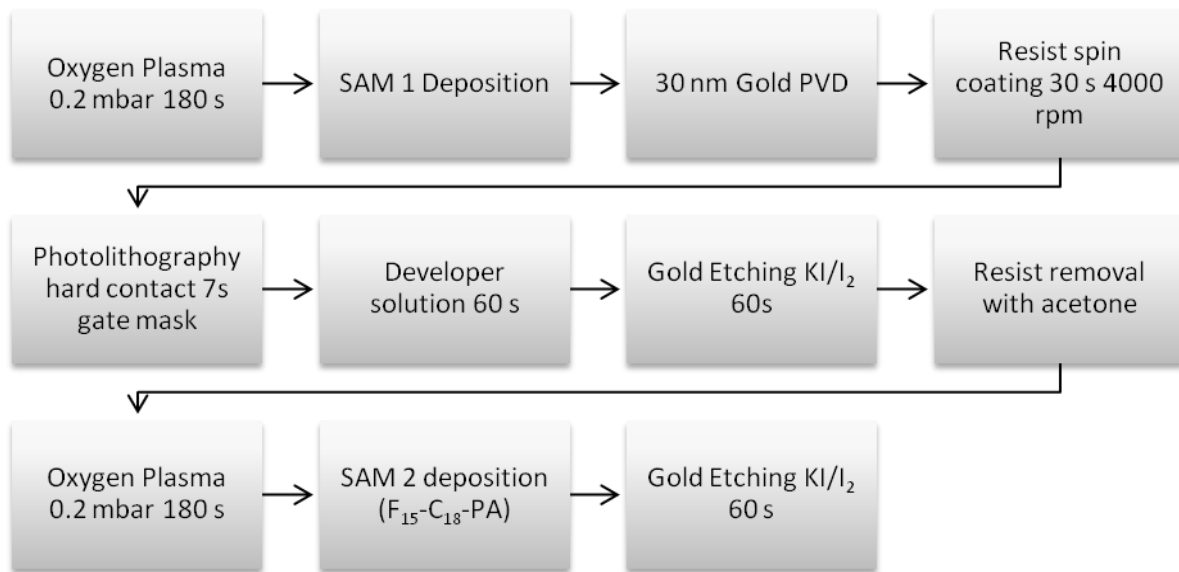


Figure S2. Process chain for fabrication of in-plane patterned substrates.

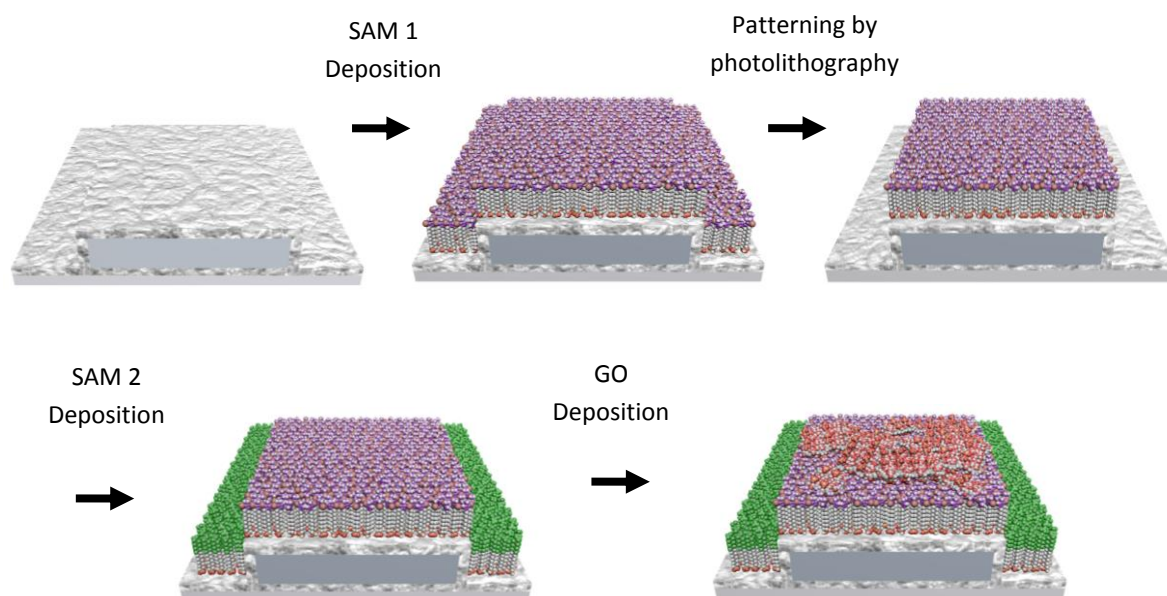


Figure S3. Schematic fabrication process of patterned SAM on aluminum electrode.

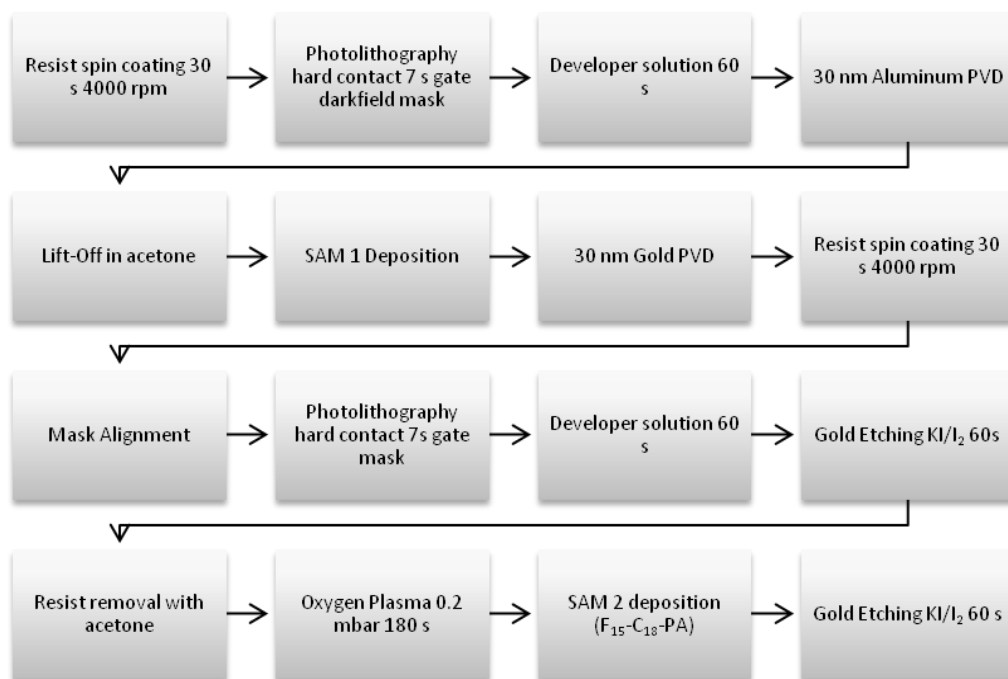


Figure S4. Process chain for fabrication of patterned SAMs on aluminum electrodes.

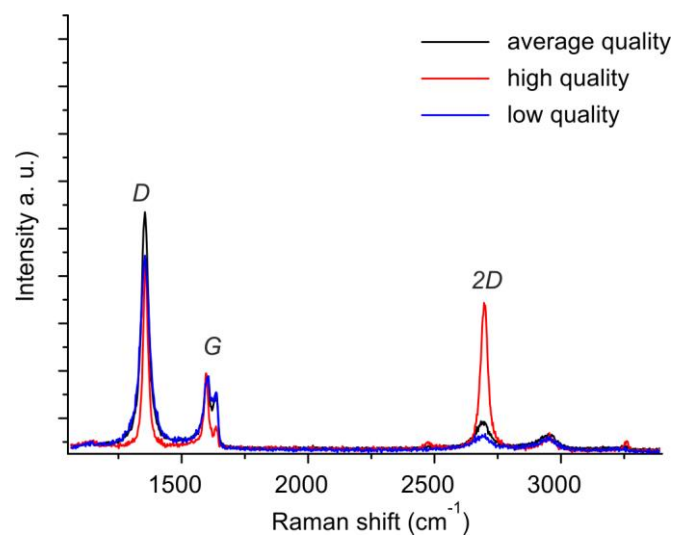


Figure S5. a) Exemplary Raman spectra of rGO of different quality. Black: average quality with $\Gamma_{2D} = 59.7 \text{ cm}^{-1}$; red: high quality with $\Gamma_{2D} = 32.5 \text{ cm}^{-1}$ and blue: low quality with $\Gamma_{2D} = 63.9 \text{ cm}^{-1}$.

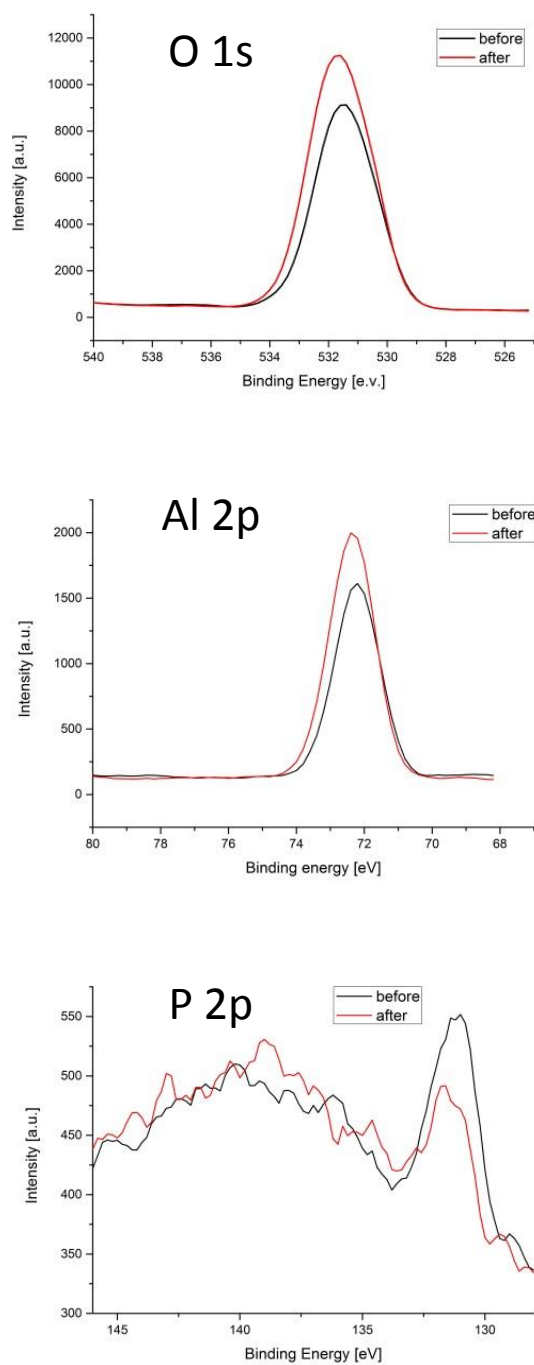


Figure S6. XPS detail spectra of MIM⁺-C₁₂-PA SAM layer before and after the treatment with reduction agents HI/TFA.

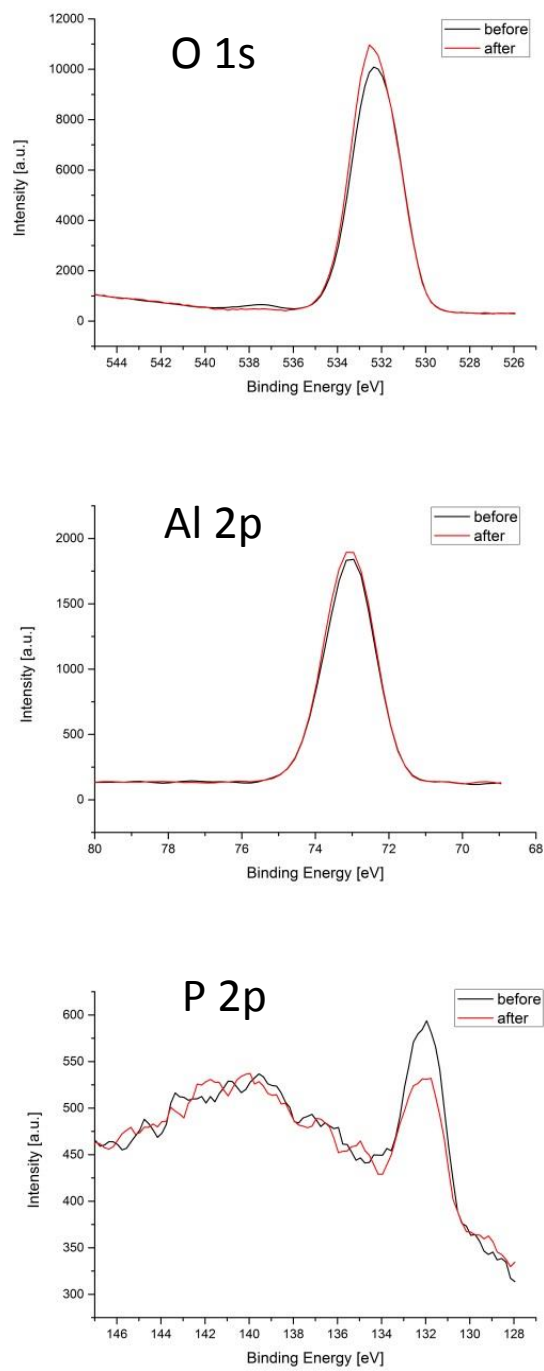
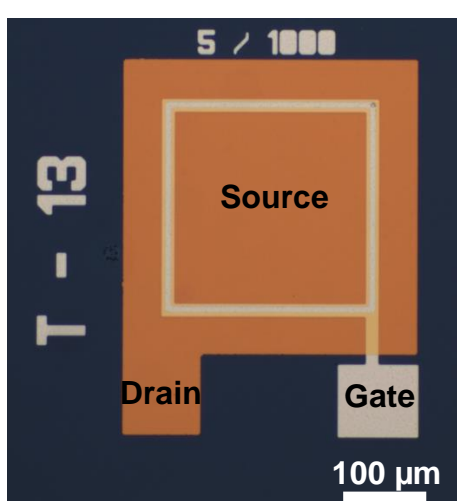
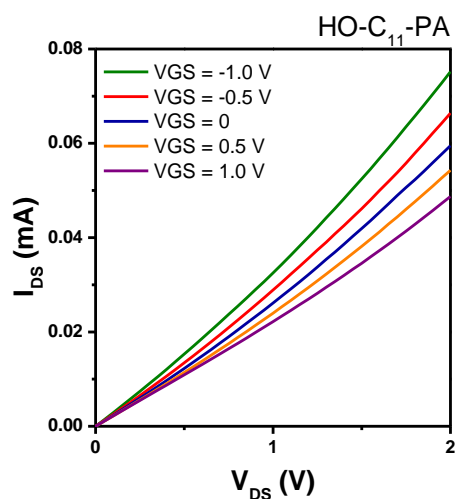


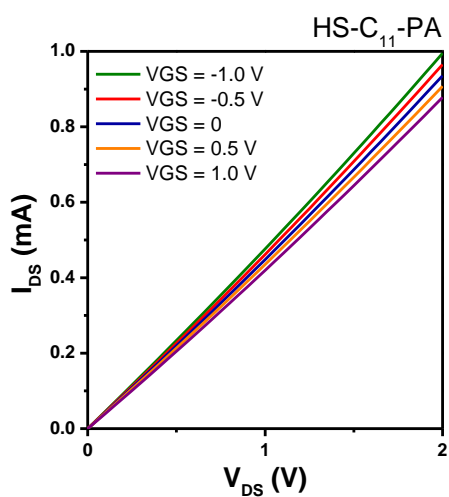
Figure S7. XPS detail spectra of NH_3^+ - C_{12} -PA SAM layer before and after the treatment with reduction agents HI/TFA.



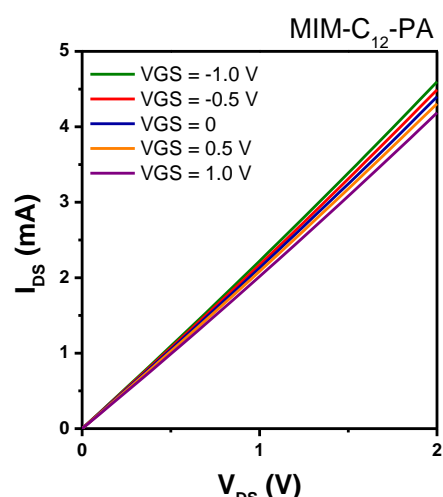
(a)



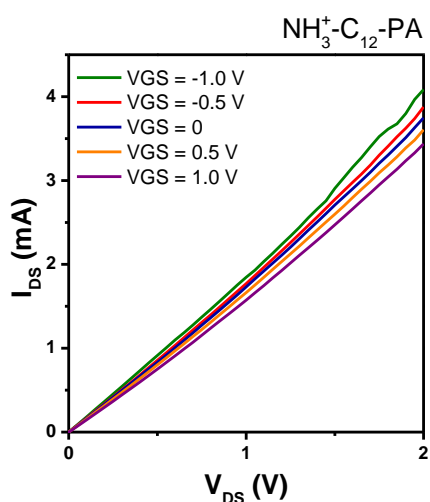
(b)



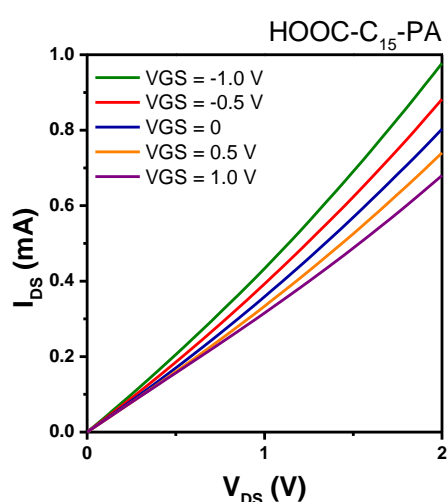
(c)



(d)



(e)



(f)

Figure S8. a) Optical images of the transistor, and output curves of transistors based on different SAMs, b) HO-C₁₁-PA, c) HS-C₁₂-PA, d) MIM⁺-C₁₂-PA, e) NH₃⁺-C₁₂-PA, and f) HOOC-C₁₅-PA.

References

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