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ADVANCED FUNCTIONAL MATERIALS

Supporting Information

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Towards Integrated Molecular Electronic Devices: Characterization of Molecular Layer Integrity During Fabrication Processes

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1. Introduction

This document contains supplemental supporting data that is referred to in the main text. J-V curves, Raman and XPS spectra, and AFM measurements are included.

2. J-V curves for Cu and Au Junctions

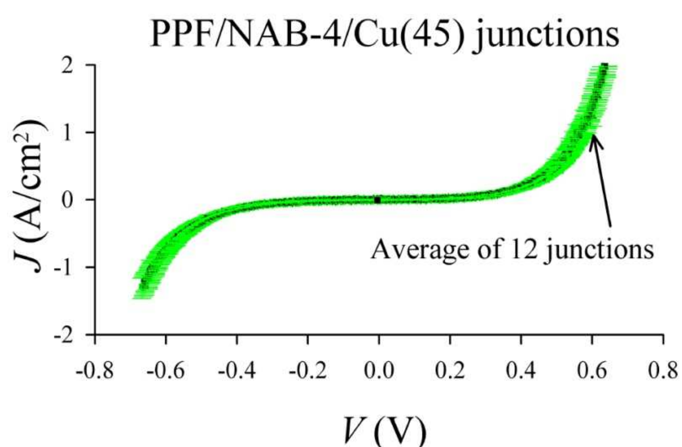


Figure S-1. The average *J-V* curve of 12 Si/SiO_2/PPF/NAB/Cu(45) junctions (black curve) with the error green bar (± 1 standard deviation) shown.

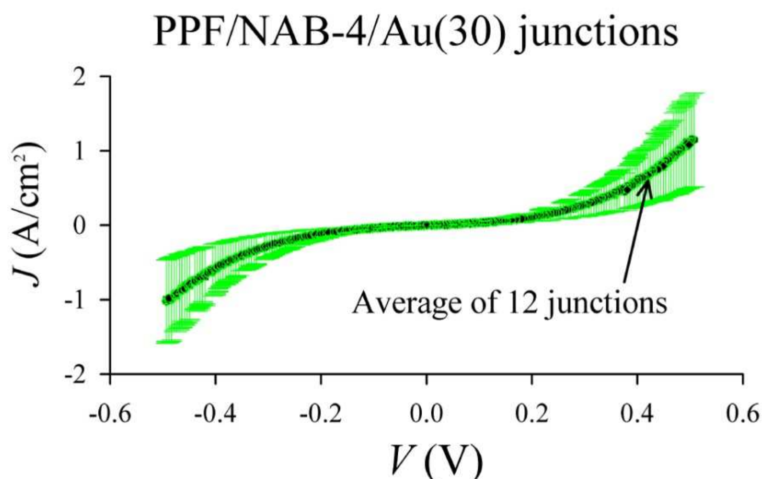


Figure S-2. The average *J-V* curve of 12 Si/SiO_2/PPF/NAB/Au(30) junctions (black curve) with the error green bar (± 1 standard deviation) shown.

3. Supplemental Raman Spectroscopy

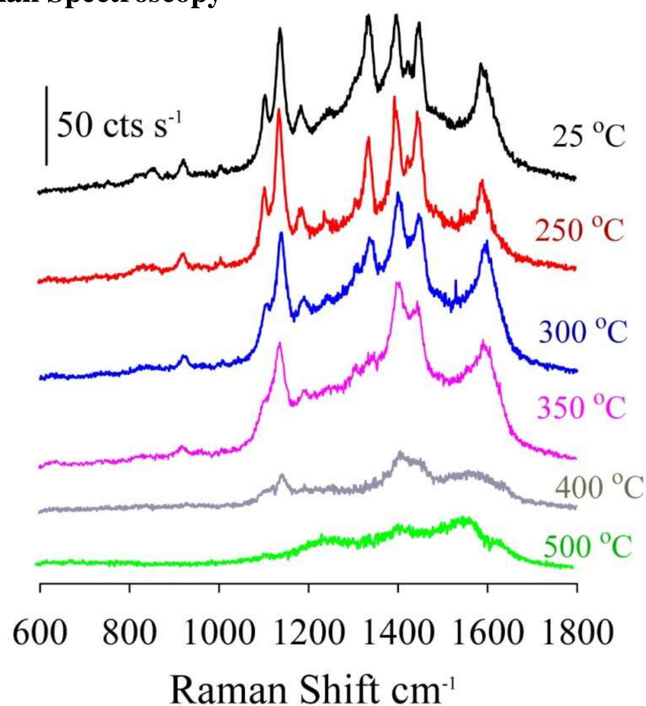


Figure S-3. Raman Spectra of Si/SiO_2/PPF/NAB after heating the sample for 30 min in Ar gas for the indicated temperature.

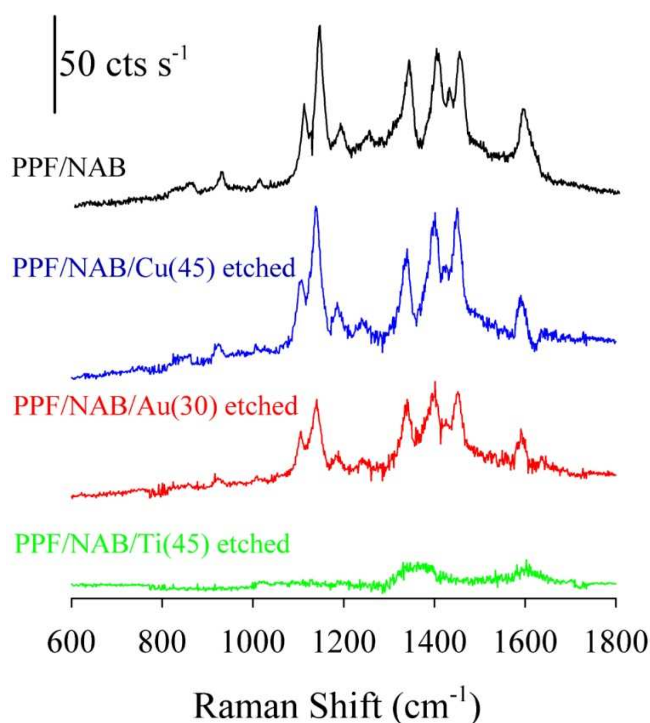
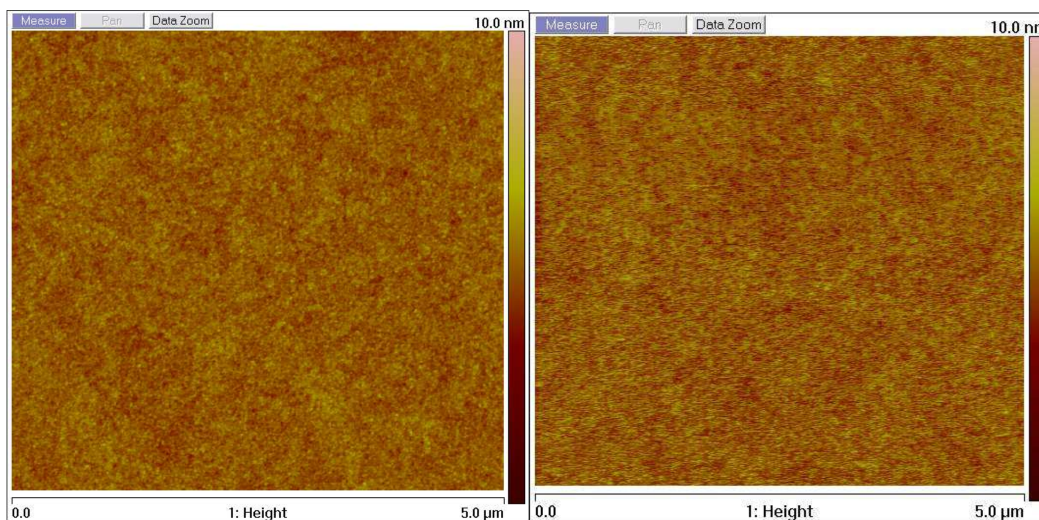


Figure S-4. Raman Spectra of Si/SiO_2/PPF/NAB initially and after etching Cu(45) Au(30), and Ti(45).

4. Supplemental AFM Images



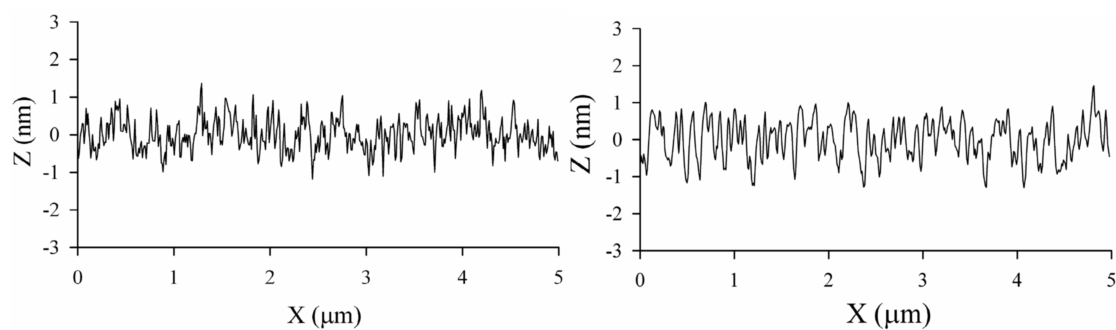


Figure S-5. 5 μm x 5 μm tapping mode AFM images of **(A)** PPF (rms ~ 0.44 nm) and **(B)** PPF/NAB (rms ~ 0.46 nm).

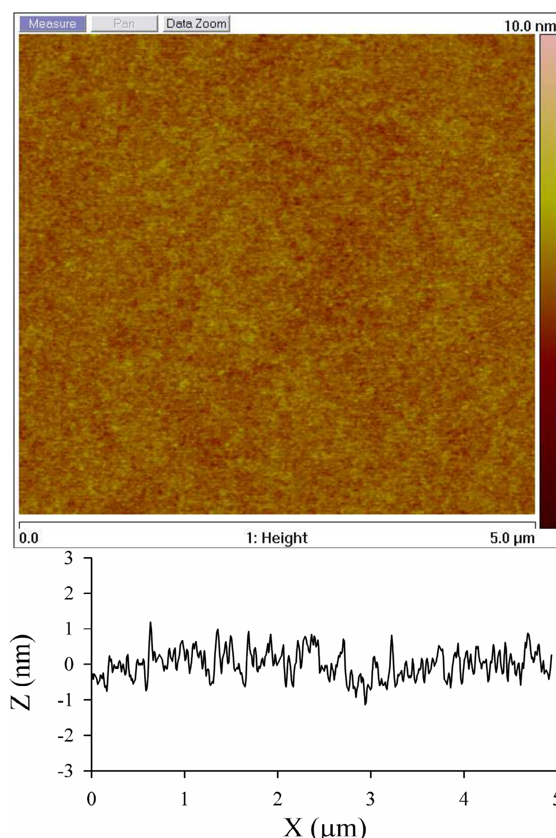


Figure S-6. Tapping mode AFM scan of Si/SiO_2/PPF/NAB after immersion in Au etchant (KI/I_2) for 60 seconds, the scanned area is 5 µm x 5µm and rms ~ 0.37 nm.

5. Supplemental XPS

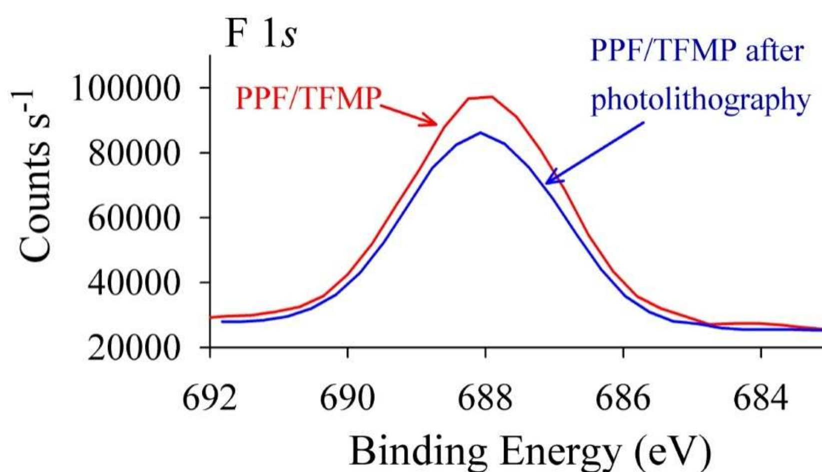


Figure S-7. High-resolution XPS spectra of F*1s* region of Si/SiO_2/PPF/TFMP-4 as before (red curve), and after (blue curve) complete photolithographic process, F/C ratio initially = 0.0865 and after photolithography = 0.0862.

6. J-V Measurements of a Parylene N Selaed Device

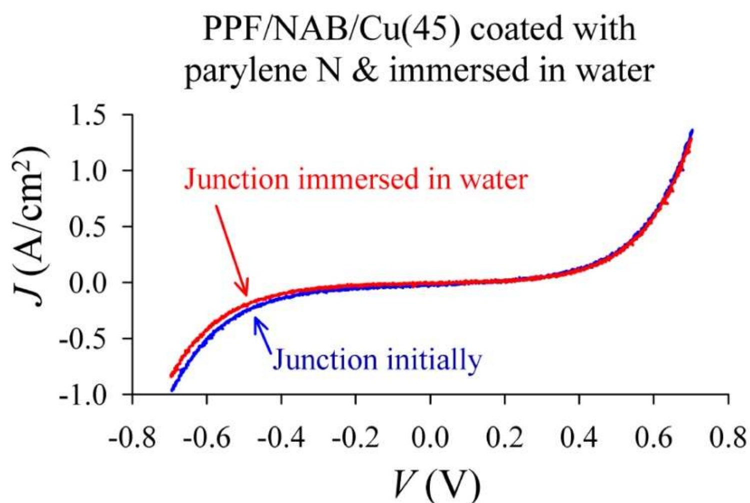


Figure S-8. *J-V* curve of Si/SiO_2/PPF/NAB/Cu(45) junction encapsulated with 0.3 μm parylene N and immersed in water for 10 minutes.

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7. Supplemental Tables

Table S-1. Ratio of Raman peaks heights relative to the Raman peak height at 1600 cm^{-1} of PPF/NAB sample initially and after heating the sample to 400 ^{o}C in vacuum (~2 x 10^{-6} torr).

Raman peak(cm^{-1})	**Peak Ratio Initially Relative to Raman Peak at 1600 cm^{-1}**	**Peak Ratio after Heating Relative to Raman Peak at 1600 cm^{-1}**
1140	1.32	1.39
1339	0.77	0.95
1401	0.83	0.72
1450	1.22	1.33

Table S-2. The reduction of Raman peak intensity at 1600 cm^{-1} and the ratios for 1402/1450 cm^{-1} (azo stretches) before and after top contact deposition for PPF/NAB samples.

Top Metal Contact	% reduction in Raman peak height at 1600 cm^{-1}	Initial 1402/1450 cm^{-1} intensity ratio	1402/1450 cm^{-1} intensity ratio after metal deposition
Cu (45)	9.8%	0.86	0.77
Au (30)	3.8%	0.88	0.74
Ti (45)	63%	0.92	0.89
Pt (30)	61%	0.92	0.92