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


Supporting Information for:

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/SiO₂/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/SiO₂/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 $5 \mu$m x $5 \mu$m and rms ~ 0.37 nm.

5. Supplemental XPS
Figure S-7. High-resolution XPS spectra of F/\text{s} 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.

![J-V curve of Si/SiO₂/PPF/NAB/Cu(45) junction encapsulated with 0.3 µm parylene N and immersed in water](image)

**Figure S-8.** $J-V$ curve of Si/SiO₂/PPF/NAB/Cu(45) junction encapsulated with 0.3 µm parylene N and immersed in water for 10 minutes.
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 °C in vacuum (≈2 x 10\(^{-6}\) torr).

<table>
<thead>
<tr>
<th>Raman peak(cm(^{-1}))</th>
<th>Peak Ratio Initially Relative to Raman Peak at 1600 cm(^{-1})</th>
<th>Peak Ratio after Heating Relative to Raman Peak at 1600 cm(^{-1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>1140</td>
<td>1.32</td>
<td>1.39</td>
</tr>
<tr>
<td>1339</td>
<td>0.77</td>
<td>0.95</td>
</tr>
<tr>
<td>1401</td>
<td>0.83</td>
<td>0.72</td>
</tr>
<tr>
<td>1450</td>
<td>1.22</td>
<td>1.33</td>
</tr>
</tbody>
</table>

**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.

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