Facile and scalable design of light-emitting and ROS-generating hybrid materials made of polyurea gels embedding a molybdenum cluster-based salt

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Table S1. Characteristics of the Hydrogen-bonded carbonyl bands in the FTIR Spectra (amide I region) of the polyurea containing different amounts of Mo cluster

<table>
<thead>
<tr>
<th>Cluster content</th>
<th>H-bond C=O band (d)</th>
<th>isocyanurate ring</th>
<th>H-bond C=O band (d)</th>
<th>H-bond C=O band (o)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>freq (cm⁻¹)</td>
<td>width (cm⁻¹)</td>
<td>freq (cm⁻¹)</td>
<td>width (cm⁻¹)</td>
</tr>
<tr>
<td>0 (PUr)</td>
<td>1716</td>
<td>16.7</td>
<td>1689</td>
<td>20.5</td>
</tr>
<tr>
<td>1 (PUr-1)</td>
<td>1717</td>
<td>20.7</td>
<td>1689</td>
<td>20.5</td>
</tr>
<tr>
<td>3 (PUr-3)</td>
<td>1717</td>
<td>18.6</td>
<td>1689</td>
<td>20.2</td>
</tr>
<tr>
<td>5 (PUr-5)</td>
<td>1715</td>
<td>27.5</td>
<td>1689</td>
<td>21.1</td>
</tr>
<tr>
<td>10 (PUr-10)</td>
<td>1716</td>
<td>18.3</td>
<td>1689</td>
<td>20.5</td>
</tr>
</tbody>
</table>

*d = disordered, o = ordered, width = full width measured at half-height
FIGURE S1: FTIR spectra and corresponding Gaussian curve-fits of the amide I region of unloaded polyurea-PUr.

FIGURE S2: FTIR spectra and corresponding Gaussian curve-fits of the amide I region of loaded polyurea containing (a) 1 wt%, (b) 3 wt%, (c) 5 wt%, (d) 10 wt% of Mo cluster respectively.
FIGURE S3: Intensity maps of Mo (first column), Br (second column) and Cs (third column) collected by confocal micro-X-ray fluorescence imaging for loaded PUr membrane containing (a) 3 wt% and (b) 5 wt% of Cs$_2$Mo$_6$Br$_{14}$ cluster.

Figure S4. Emission vs excitation map of PUr-1
**Figure S5.** Emission decay map recorded at $\lambda_{\text{exc}} = 375$ nm for PUr-1.

**Figure S6.** Integrated emission decay profile recorded for PUr-1 ($\lambda_{\text{exc}} = 375$ nm) and residual plot of the calculated fit.
Figure S7. Emission vs excitation map of PUr-3.

Figure S8. Emission decay map recorded at $\lambda_{\text{exc}} = 375$ nm for PUr-3.
Figure S9. Integrated emission decay profile recorded for PUr-3 ($\lambda_{exc} = 375$ nm) and residual plot of the calculated fit.

Figure S10. Emission vs excitation map of PUr-5.
Figure S11. Emission decay map recorded at $\lambda_{\text{exc}} = 375$ nm for PUr-5.

Figure S12. Integrated emission decay profile recorded for PUr-5 ($\lambda_{\text{exc}} =375$ nm) and residual plot of the calculated fit.
**Figure S13.** Emission vs excitation map of PUr-10.

**Figure S14.** Emission decay map recorded at $\lambda_{\text{exc}} = 375$ nm for PUr-10.
Figure S15. Integrated emission decay profile recorded for PUr-10 ($\lambda_{\text{exc}} = 375$ nm) and residual plot of the calculated fit.

Figure S16. $1\Delta_g$ O$_2$ emission spectra observed for PUr-1 (black), PUr-3 (red), PUr-5 (green) and PUr-10 (blue) by exciting samples at 375 nm.