Supporting Information

Functional group effect on flame retardancy, thermal, and mechanical properties of organophosphorus-based magnesium oxysulfate whiskers as flame retardant in polypropylene

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X-ray diffraction was employed to analyze the crystal structure of MOSw and DDPMOSw. From Figure 2, both patterns of MOSw and DDPMOSw presented uniform diffraction peaks at 2θ around 12°, 17°, 22°, 30°, 34°, 40° and 46°, assigned to (201), (202), (203), (111), (601), (114) and (513) crystal faces, respectively. Above all, it was confirmed that functionalization occurred only on the surface of MOSw without altering its crystal structure. However, the intensity of some peaks decreases significantly after DDP modification. This is attributed to the amorphous coating layer on the surface of MOSw, as shown in the TEM micrographs, suggesting that the DDP was well-coated on the whole surface of the whiskers. As such, the surface of MOSw turned into hydrophobicity.
**Table S1.** The Element Content Analyses of MOSw and DDPMOSw by XPS.

<table>
<thead>
<tr>
<th>Element</th>
<th>Unmodified MOSw (%)</th>
<th>DDPMOSw (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mg</td>
<td>18.07</td>
<td>14.54</td>
</tr>
<tr>
<td>O</td>
<td>49.48</td>
<td>40.14</td>
</tr>
<tr>
<td>S</td>
<td>4.37</td>
<td>2.12</td>
</tr>
<tr>
<td>P</td>
<td>0</td>
<td>1.97</td>
</tr>
<tr>
<td>C</td>
<td>28.08</td>
<td>41.23</td>
</tr>
</tbody>
</table>

**Fig S2.** Water contact angle of MOSw (a) and DDPMOSw (b).

From Figure S2, it was clearly that the water contact angle of MOSw were 0 since complete wetting surface of hydrophilic MOSw. However, the water contact angle remarkably increased to to 131.3°, indicating that the surface of MOSw had good hydrophobicity after the surface modification.
As shown in Figure S3, although DDPMOSw distributed evenly in the PP matrix, the surface of naked whiskers was still as smooth as usual. Hence, it was considered that DDP functionalization only improved the dispersity of MOSw, but not enhance the compatibility between MOSw and the PP matrix.

![SEM micrographs of PP/DDPMOSw composite in high resolution.](image1.png)

**Fig S3.** SEM micrographs of PP/DDPMOSw composite in high resolution.

![TG curves of MOSw and DDPMOSw.](image2.png)

**Fig S4.** TG curves of MOSw and DDPMOSw.
TG analysis was employed to investigate the thermal stability of the MOSw and DDPMOSw in an atmosphere of N₂, as shown in Figure S4. For MOSw, there were three steps of decomposition from 250 °C to 888 °C. The weight loss from 250 °C to 282 °C was about 8.4 wt%, corresponding to the release of two crystal water molecules of 5Mg(OH)₂·MgSO₄·2H₂O. The weight loss from 371 °C to 411 °C was about 19.4 wt%, due to the dehydration of 5Mg(OH)₂·MgSO₄. The weight loss from 848 °C to 888 °C was about 18.01%, attributed to the desulfation (SO₃) of 5MgO·MgSO₄. Obviously, DDPMOSw showed almost superimposed curves with MOSw in the first two steps, indicating that DDP seldom effected the dehydration process of MOSw. Furthermore, the weight loss of DDPMOSw from 370 °C to 412 °C was greater than that of MOSw, probably due to the decomposition of DDP coating. This behavior was more clear in the third decomposition step of DDPMOSw, which may be beneficial for improving the flame retardant properties of the polymers/MOSw composites.

**Scheme S1.** Schematic illustration of the mechanism for the flame resistance of the PP/MOSw composite.