MATERIAL SUPLEMENTAR

Lewis acid sites of Mg$^{2+}$-modified polystyrene sulfonic acid resin catalysys for synthesis of dibutyl succinate

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The D002, Cl-D002 and Mg-Cl-D002 were characterized by EDS to determine the elemental composition (Figure 1S). In the EDS spectrum, Mg, and Cl peaks were observed.

a)

b)
The optimum monomer structures (Figure 2S) of D002, Cl-D002 and MgSO₄-Cl-D002 have been studied using density functional theory methods at the B3LYP/6-311G(d,p) computational level (Table 1S), which agree in general with the structure reported in literature.¹ ² The total energy of the Cl-D002 and MgSO₄-Cl-D002 were lower than observed for the D002, so the optimum monomer structures of Cl-D002 and MgSO₄-Cl-D002 may exist.³
Figure 2S. The optimum structure of: a) D002; b) Cl-D002; c) D002Mg-Cl-D002

Table 1S. The total energies of resins

<table>
<thead>
<tr>
<th>B3LYP/6-311G(d,p)</th>
<th>Total energies(a.u.)</th>
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</thead>
<tbody>
<tr>
<td>D002</td>
<td>-933.61023</td>
</tr>
<tr>
<td>Cl-D002</td>
<td>-1393.22736</td>
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<tr>
<td>Mg-Cl-D002</td>
<td>-2985.43249</td>
</tr>
</tbody>
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REFERENCES