

Supporting Information

Nanosheet magnesium oxide as an effective catalyst on the synthesis of diethyl carbonate from ethyl carbamate and ethanol

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S1. Models:

The optimized geometrical structure of (a) MgO (100) surface ; (b) EC molecule; (c) ethanol molecule are as follows. For clarity, the main atoms of the adsorbed molecules are labeled and the oxygen atom of MgO is labeled as O_M, as shown in Fig. S1.

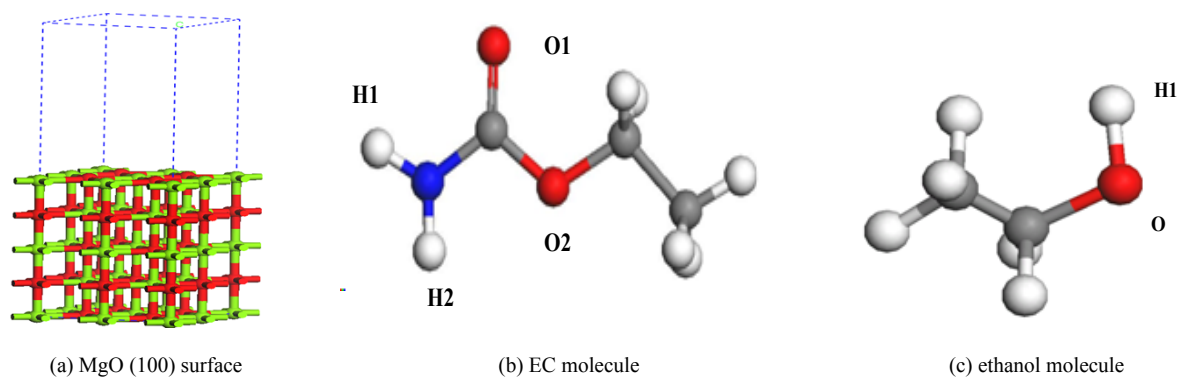


Fig. S1 Optimized geometrical structure of (a) MgO (100) surface, (b) EC molecule, and (c) ethanol molecule

S2. Mastersizer 2000

Particle size of MgO-SC-450 sample was analyzed using particle size analyzer model Mastersizer 2000. The volume mean particle diameter (d_{50}) was used to express the mean particle size of MgO-SC-450. It means that the volume of particles below d_{50} size is half of the total volume of the sample. The result yields an average particle size of 21 μm (about 600 mesh). In this case, Mastersizer 2000 measures the agglomerations instead of crystallites.

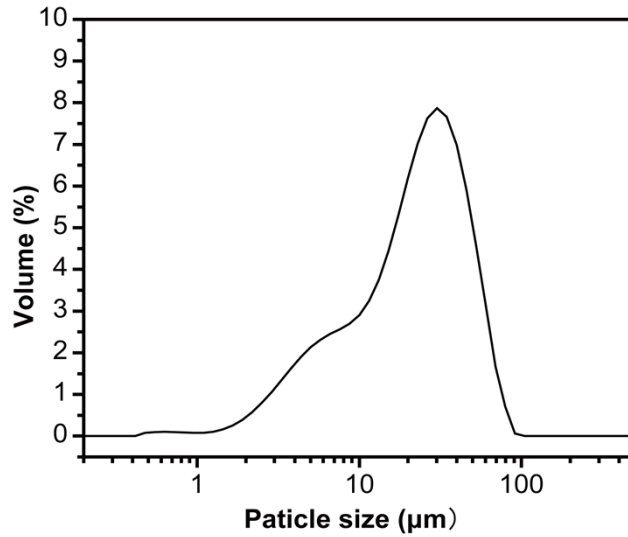


Fig. S2 Size distribution of MgO-SC-450.