

### Description of Additional Supplementary Files

**Supplementary Data 1** - This file encompasses the atomic coordinates for all pertinent computational models utilized in this study.

In-MOF-GO: The atomic coordinates of the computational models of In-MOF/GO.

In-MOF-GO-CO<sub>2</sub>: The atomic coordinates of the computational models of In-MOF/GO-CO<sub>2</sub>.

In-MOF-GO-COOH: The atomic coordinates of the computational models of In-MOF/GO-COOH.

In-MOF-GO-CO: The atomic coordinates of the computational models of In-MOF/GO-CO.

In-MOF-CO<sub>2</sub>: The atomic coordinates of the computational models of In-MOF-CO<sub>2</sub>.