## Thermal Conductivity of 2-D Covalent Organic Framework and

## Enhancing Using Fullerene 3-D Self-assembly: A Molecular

## **Dynamics Simulation**

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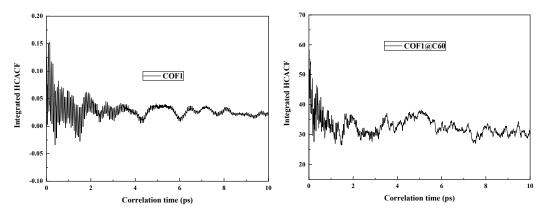
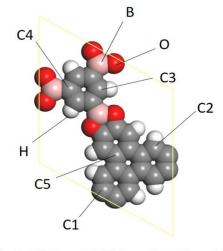


Figure S1. Time-dependent integral HCACF of (a) COF-1 and (b) C60@COF-1.



a=b=14.974,c=3.3986,  $\alpha$ =b=90°, y=120°

Figure S2. The structural motif and atomic types of COF-6.

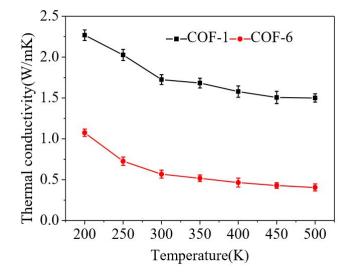


Figure S3. The MD prediction of thermal conductivity for COF-6.