Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Host and guest joining forces: a holistic approach for metal-organic frameworks in nonlinear optics

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1. Structure of MOF-177

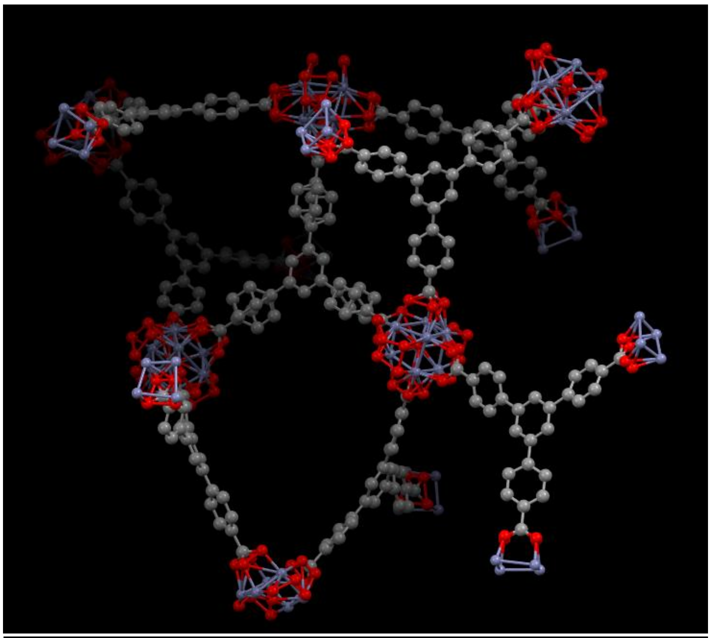

Figure S1. Structure of MOF-177.[1,2]

2. FT-IR spectra obtained from C_{60}⊂MOF-177, Li@C_{60}⊂MOF-177 and precursor compounds

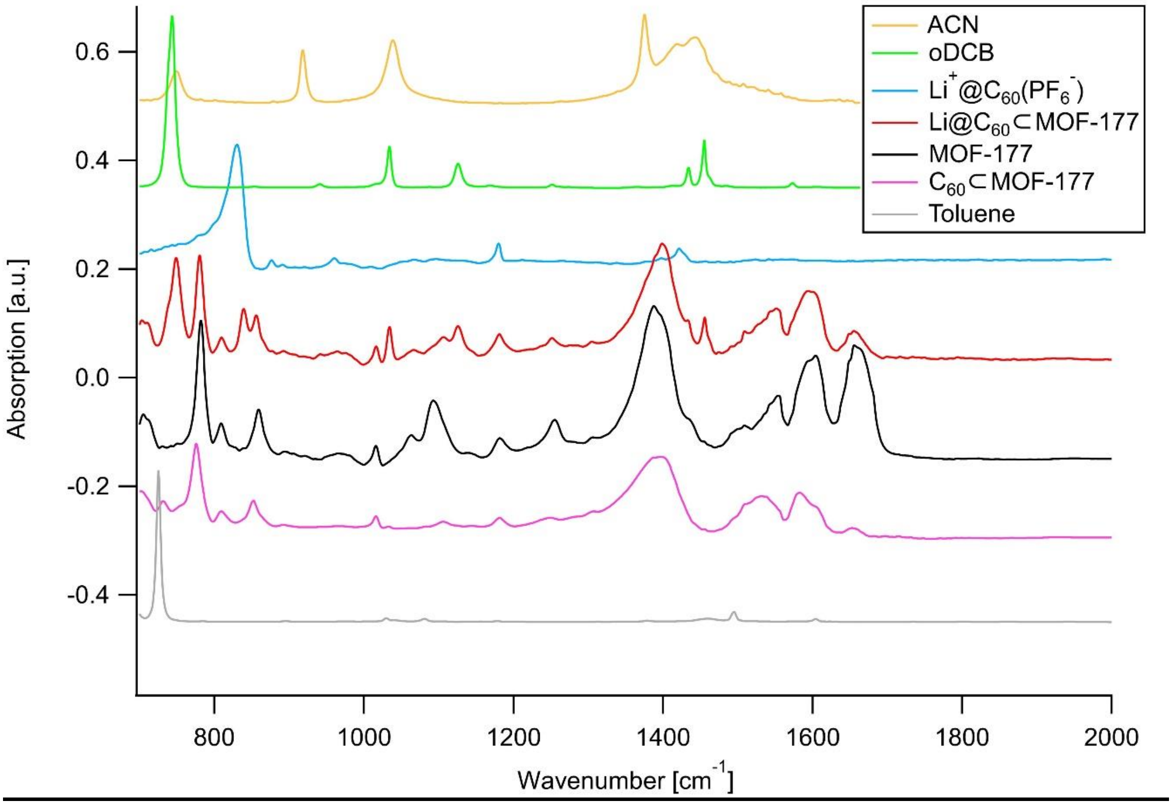

Figure S2. FTIR obtained from toluene (grey), C_{60}⊂MOF-177 (pink), MOF-177 (black), Li@C_{60}⊂MOF-177 (red), Li^+@C_{60}(PF_6^-) powder (blue), oDCB (green) and ACN (orange).

3. ICP-OES measurement for lithium

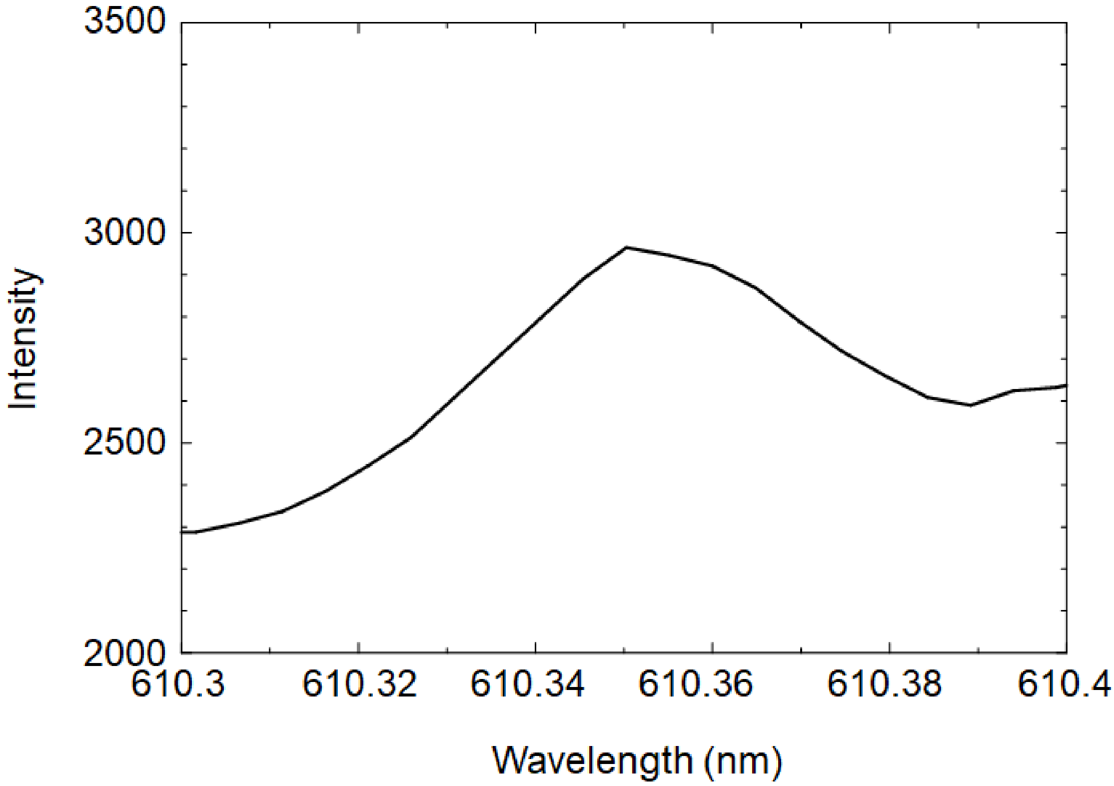

Figure S3. ICP-OES result of lithium after digesting Li@C_{60}⊂MOF-177. ICP emission from Li was observed at 610.364 nm.

4. Thermogravimetry for determination of Li@C_{60} loading

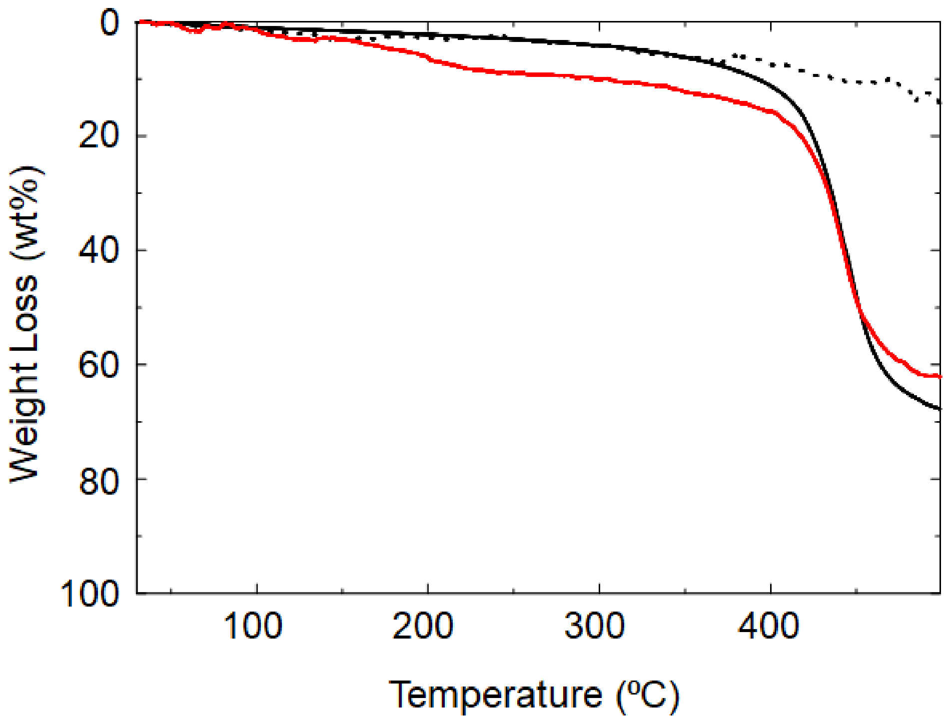

Figure S4. Thermogravimetry of Li@C_{60}⊂MOF-177 (red), MOF-177 (black solid) and Li@C_{60}[PF_6] (black dots).

5. Raman spectrum of Li@C60 in solution of oDCB and ACN

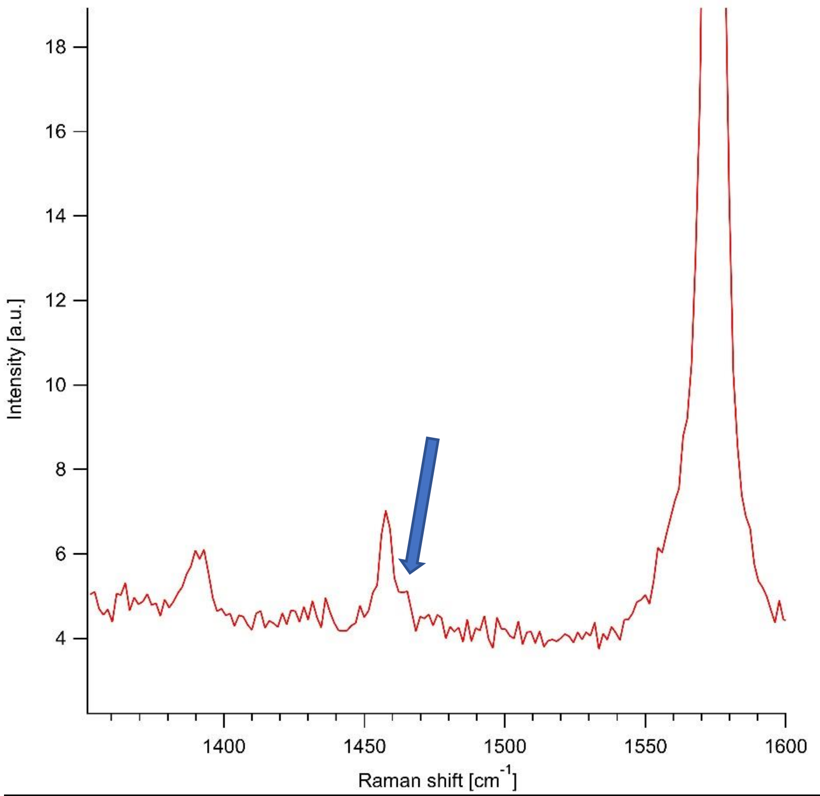

Figure S5. Raman spectrum of Li@C_{60} dissolved in a 1:1 (v:v) mixture of oDCB and ACN. The $A_g(2)$ mode of peak of C_{60} can still be observed.

6. Raman spectrum of C_{60}⊂MOF-177

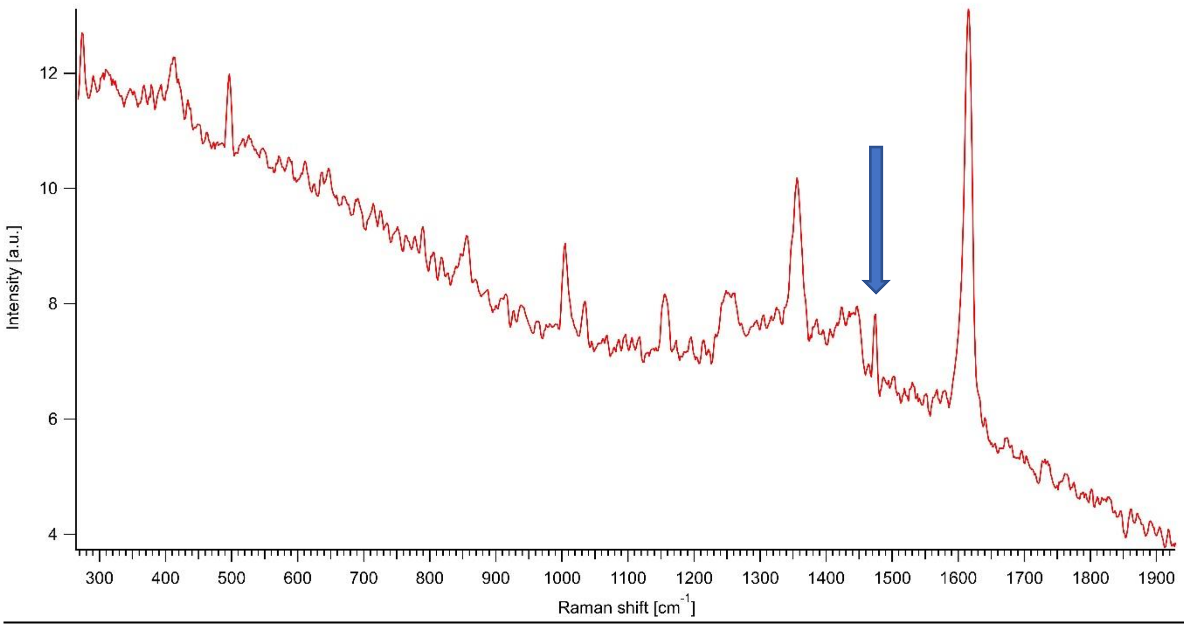

Figure S6. Raman spectrum obtained from C_{60}⊂MOF-177. The $A_g(2)$ mode of C_{60} can be clearly observed. Excited by 785 nm laser.

7. Raman spectra obtained for analysis of Zn-O bond of MOF-177

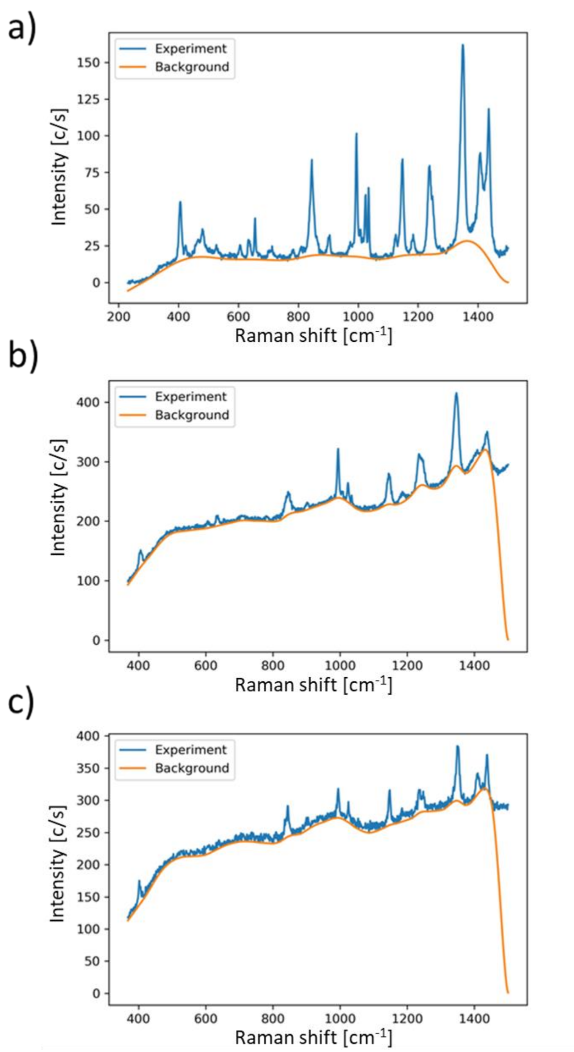

Figure S7. Raman spectra obtained from MOF-177 (a) soaked in o-dichlorobenzene/acetonitrile, (b) with accommodated C_{60} and (c) with accommodated $Li@C_{60}$. The orange line shows the background that was substracted.

8. Raman mapping obtained from C_{60}⊂MOF-177 and Li@C_{60}⊂MOF-177

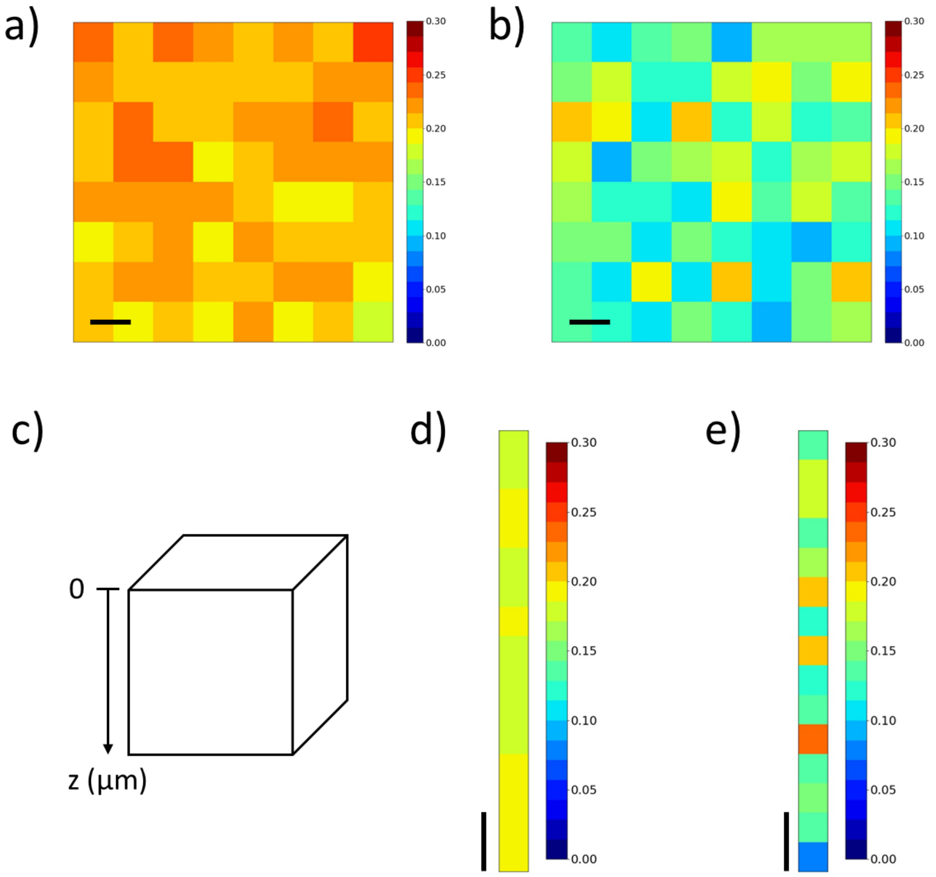

Figure S8. Raman scattering intensity x,y map of (a) C_{60}⊂MOF-177 and (b) Li@C_{60}⊂MOF-177. (c) schematic illustration to indicate z-position for the depth direction. Raman scattering intensity along the depth direction of (d) C_{60}⊂MOF-177 and (e) Li@C_{60}⊂MOF-177. The relative intensity of C_{60} (1470 cm^{-1}) against MOF-177 (1610 cm^{-1}) and Li@C_{60} (272 cm^{-1}) against MOF-177 (1360cm^{-1}) were plotted for C_{60}⊂MOF-177 and Li@C_{60}⊂MOF-177, respectively. Scale bars are 2 μm.

9. UV-vis spectrum of Li@C_{60} dissolved in 1:1 (v:v) mixture of o-dichlorobenzene and acetonitrile

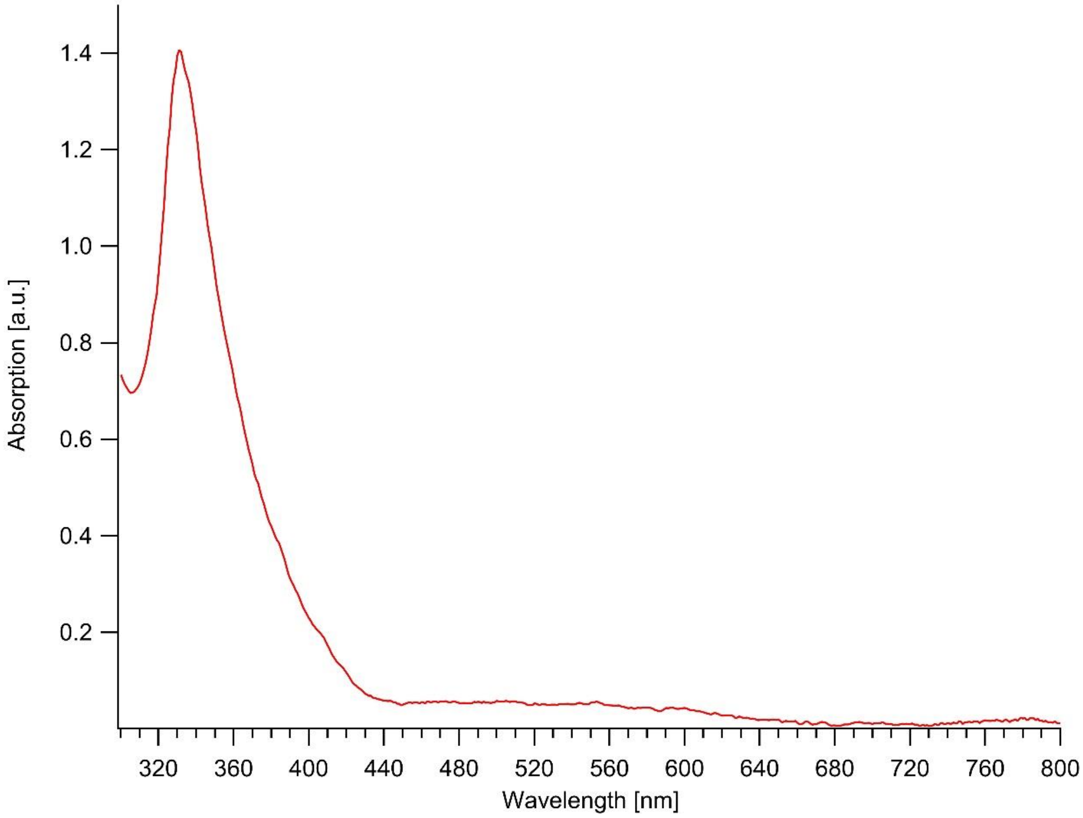

Figure S9. UV-vis spectrum of Li@C_{60} dissolved in 1:1 (v:v) mixture of o-dichlorobenzene and acetonitrile

10. SHG from MOF-177 after exposure to vacuum

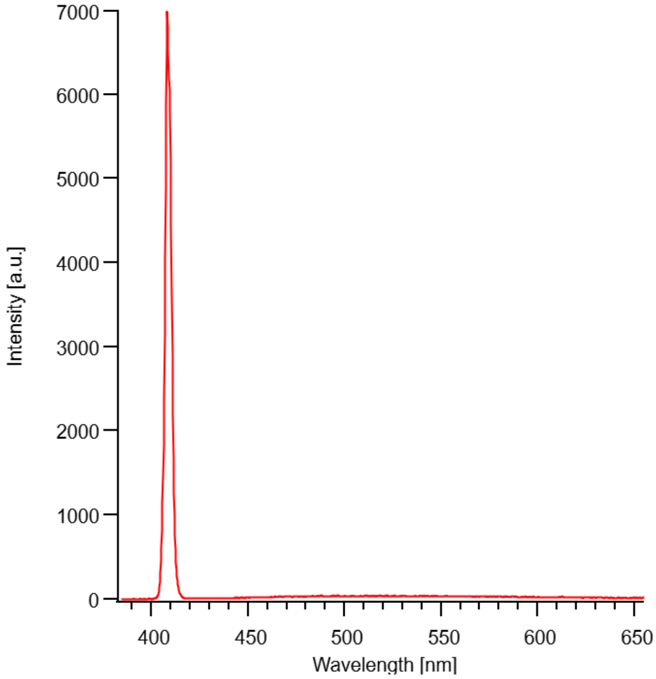

Figure S10. SHG from MOF-177 after exposure to vacuum for 30 min.

11. Correction of the polarized SHG data

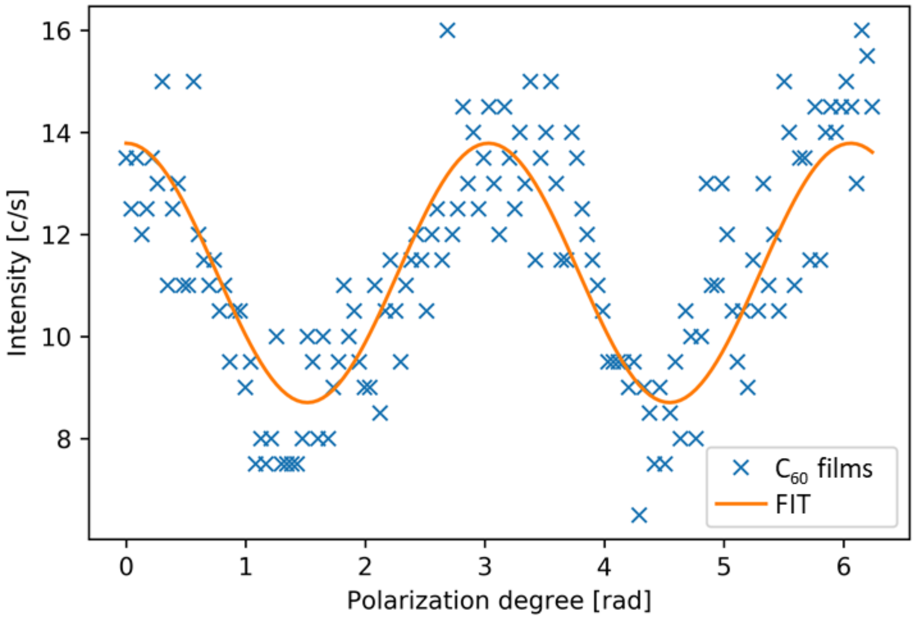

Figure S11. SHG from a C_{60} films while the polarization of the excitation beam is rotated. Excitation by 830 nm.

Several components of the microscope as well as the detection system have a polarization dependence (e.g. dichroic mirrors, grating, …). In order to account for these dependences, a C_{60} film was used. It was reported previously that the SHG emission from C_{60} films remains constant when the polarization of the excitation beam is rotated.[3]

The SHG intensity emitted from a C_{60} film upon rotation of the polarization is shown in Figure S6. The resulting data has been fitted using a cosine function. The resulting function was then normalized and the experimental data obtained from MOF-177 divided by this normalized curve to obtain the corrected data.

12. Photographs of $C_{60}\subset$MOF-177 and Li@$C_{60}\subset$MOF-177

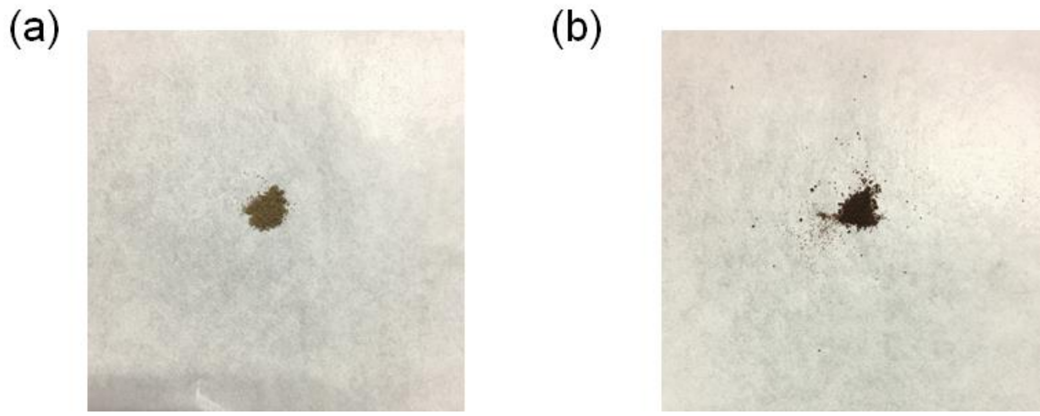

Figure S12. Photographs of (a) $C_{60}\subset$MOF-177 and (b) Li@$C_{60}\subset$MOF-177.

References

[1] H. K. Chae, D. Y. Siberio-Pérez, J. Kim, Y. Go, M. Eddaoudi, A. J. Matzger, M. O'Keeffe and O. M. Yaghi, *Nature*, 2004, 5, 523-527

[2] K. Momma and F. Izumi, *J. Appl. Crystallogr.*, 2011, 44, 1272

[3] X. K. Wang, T. G. Zhang, W. P. Lin, S. Z. Liu, G. K. Wong, M. M. Kappes, R. P. H. Chang and J. B. Ketterson, *Appl. Phys. Lett.*, 1992, 60, 810–812.