Supporting Information

Catalytic oxygen evolution from hydrogen peroxide by trans-[Co(en)$_2$Cl$_2$]@InBTB metal-organic framework catalytic system

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Table S1. The comparison of trigonal unit cell dimensions for as-prepared InBTB and various guest@InBTB MOFs.

MOFs	*a* (Å)	*b* (Å)	*c* (Å)	*V* (Å^3)	Ref.
InBTB	44.2269(19)	44.2269(19)	42.519(2)	72026(6)	[1]
trans-$[Co(en)_2Cl_2]$@InBTB	44.879(8)	44.879(8)	42.029(7)	73311(22)	This work
RD@InBTB	45.597(6)	45.597(6)	40.718(8)	73314(21)	[1]
$Ru(bpy)_3$@InBTB	44.7175(10)	44.7175(10)	42.1464(11)	72987(4)	[3]
$Ru(phen)_3$@InBTB	44.8647(7)	44.8647(7)	41.8779(8)	73000(3)	[3]
$Ru(bpz)_3$@InBTB	45.1932(4)	45.1932(4)	41.6636(5)	73694(16)	[3]

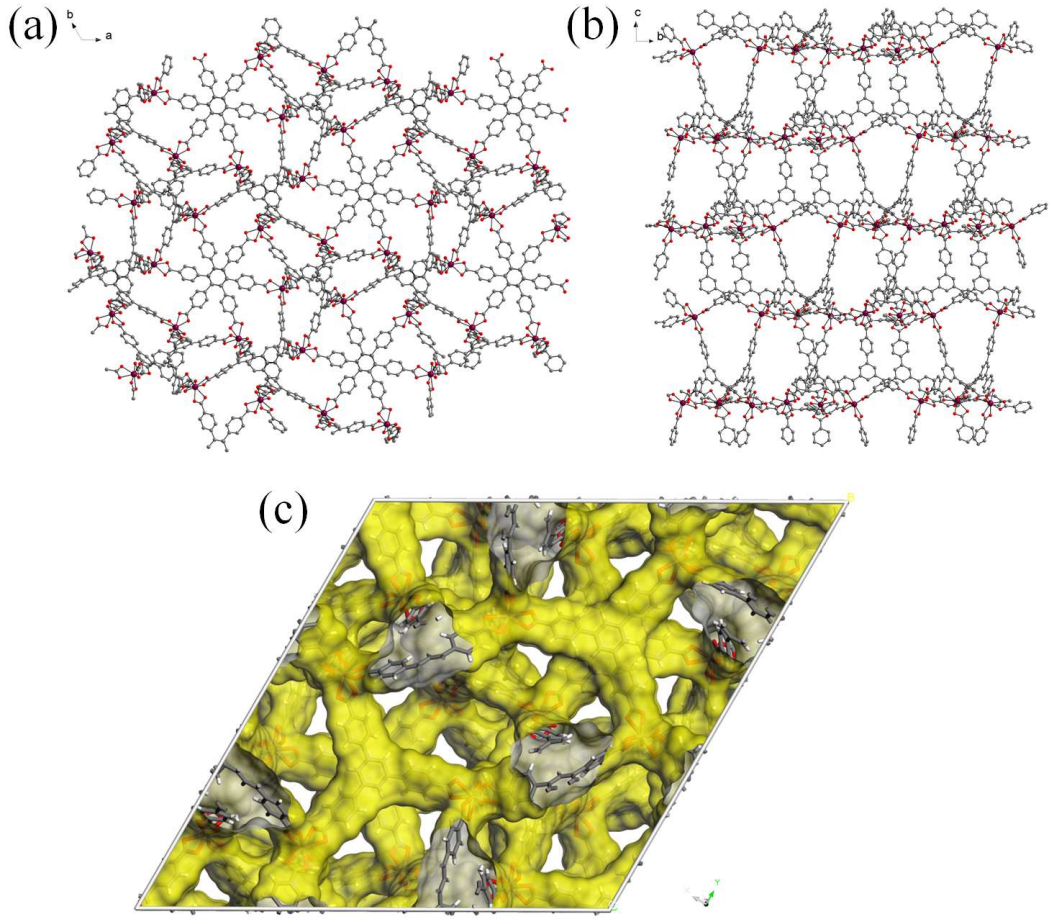

Figure S1. The crystal structure of a doubly-interpenetrated InBTB framework shown along the *c*-axis (a) and the *a*-axis (b). Hydrogen atoms are omitted for clarity. The corresponding Connolly surface (c) [1].

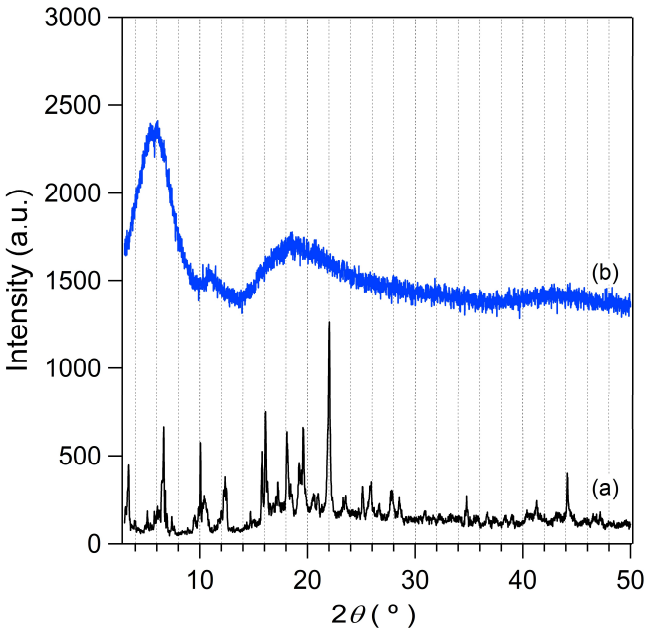

Figure S2. PXRD patterns of as-prepared InBTB (a) and *trans*-$[Co(en)_2Cl_2]$@InBTB (b).

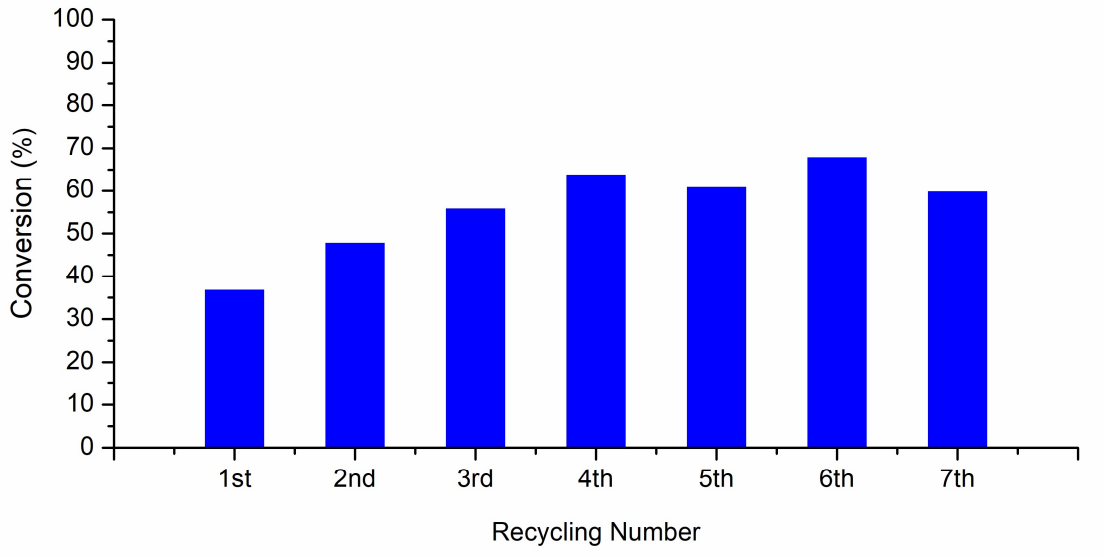

Figure S3. Recycling experimental results of H_2O_2 decomposition reaction catalyzed by *trans*-$[Co(en)_2Cl_2]$@InBTB at 40 °C.

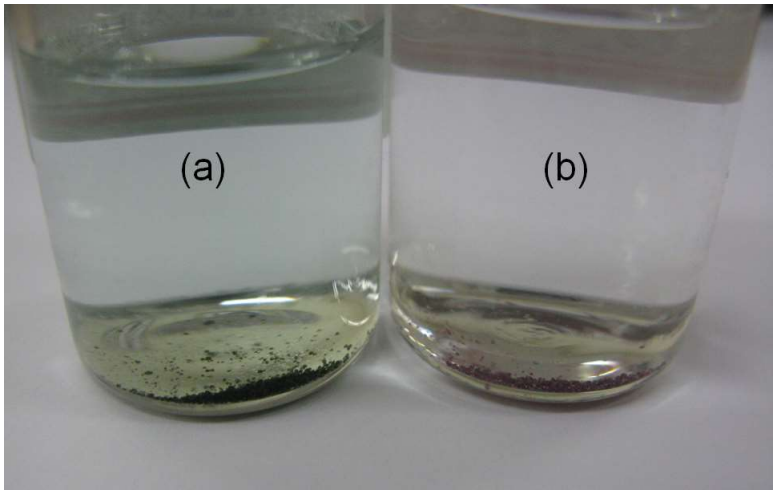

Figure S4. Digital photo images of the ethanol suspension of *trans*-$[Co(en)_2Cl_2]$@InBTB formed through the encapsulation of *trans*-$[Co(en)_2Cl_2]^+$ ion by InBTB (a) and H_2O_2-treated *trans*-$[Co(en)_2Cl_2]$@InBTB in deionized water (b).

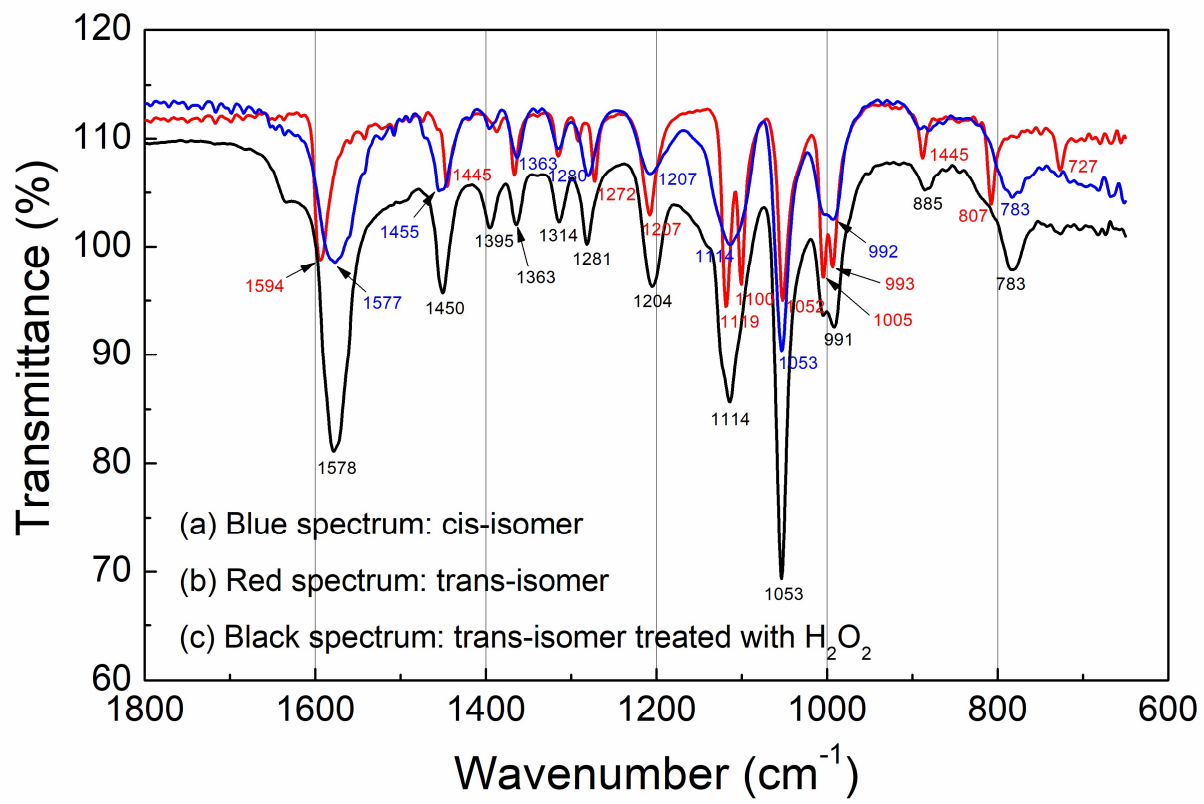

Figure S5. FT-IR spectra of *cis*-$[Co(en)_2Cl_2]Cl$ (a), *trans*-$[Co(en)_2Cl_2]Cl$ (b), and H_2O_2-treated *trans*-$[Co(en)_2Cl_2]Cl$ (c).

References

[1] E.-Y. Cho, J.-M. Gu, I.-H. Choi, W.-S. Kim, Y.-K. Hwang, S. Huh, S.-J. Kim and Y. Kim, *Cryst*. *Growth Des*., 2014, **14**, 5026-5033.

[2] J. C. Bailar, *Inorg*. *Synth*., 1946, **2**, 222-225.

[3] I.-H. Choi, S. Yoon, S. Huh, S.-J. Kim and Y. Kim, *Chem*. *Eur*. *J*., 2020, **26**, 14580-14584.