Electronic Supplementary Material (ESI) for Dalton Transactions.

In or on, a study of the influence of the binding site for TiO_2 and MIL-101(Cr)

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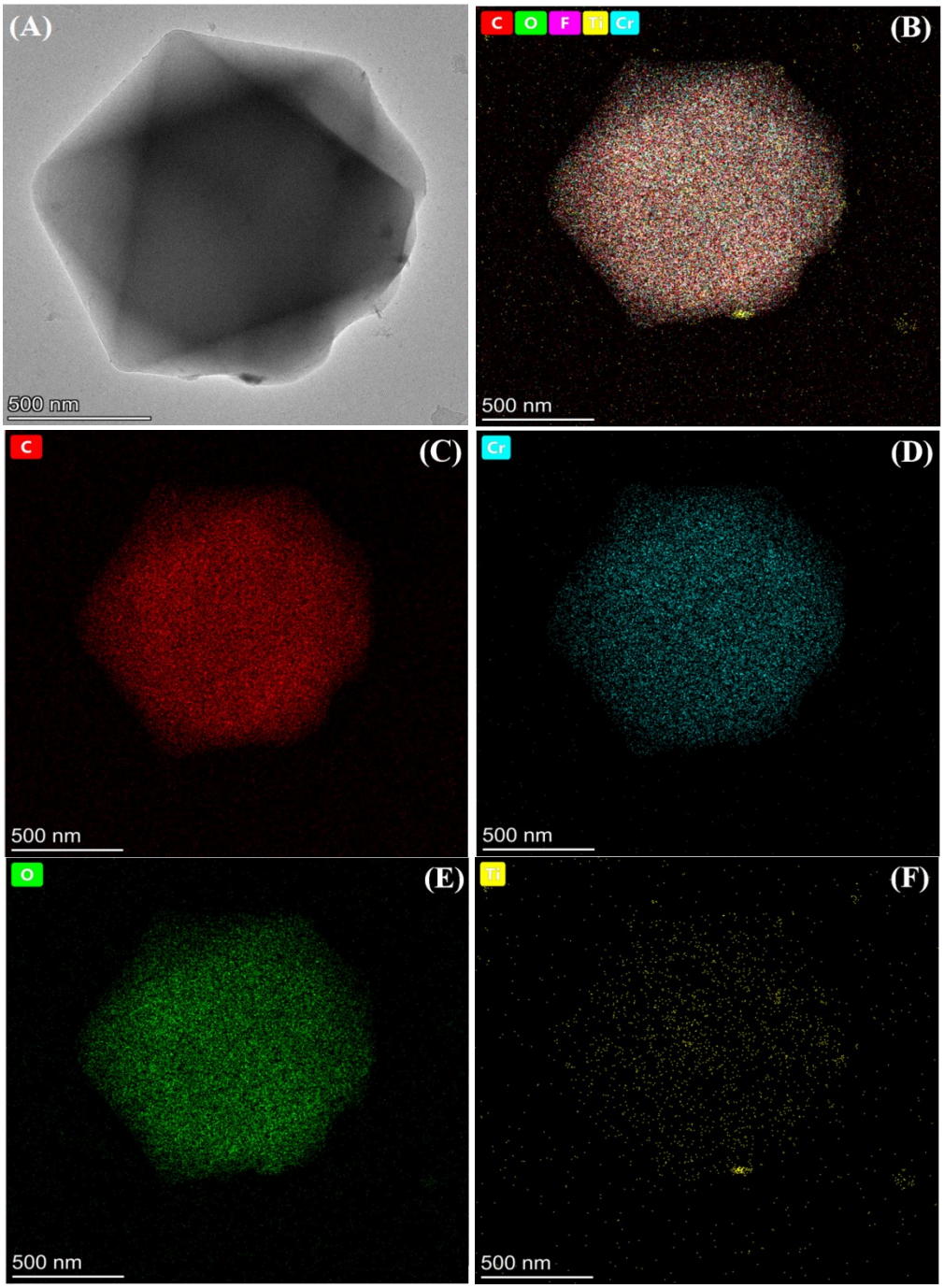
1. EDS elemental mapping



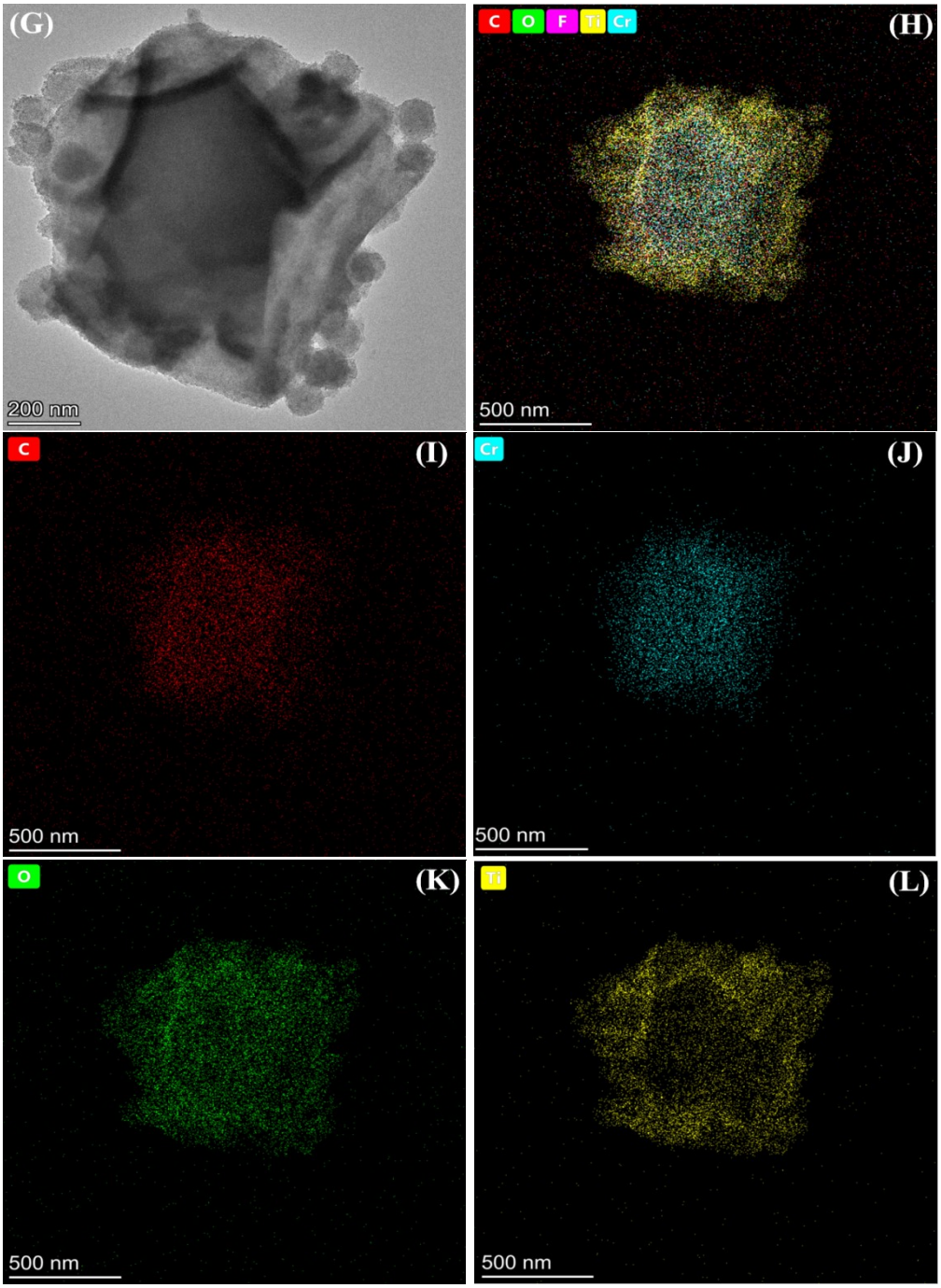


Fig. S1 (A) TEM and (B) to (F) the element distribution of TiO_2-in-MIL-101(Cr), (G)TEM and (H) to (L) the element distribution of TiO_2-on-MIL-101(Cr).

2. Fluorescence, photoelectrochemistry and electrochemistry characterization

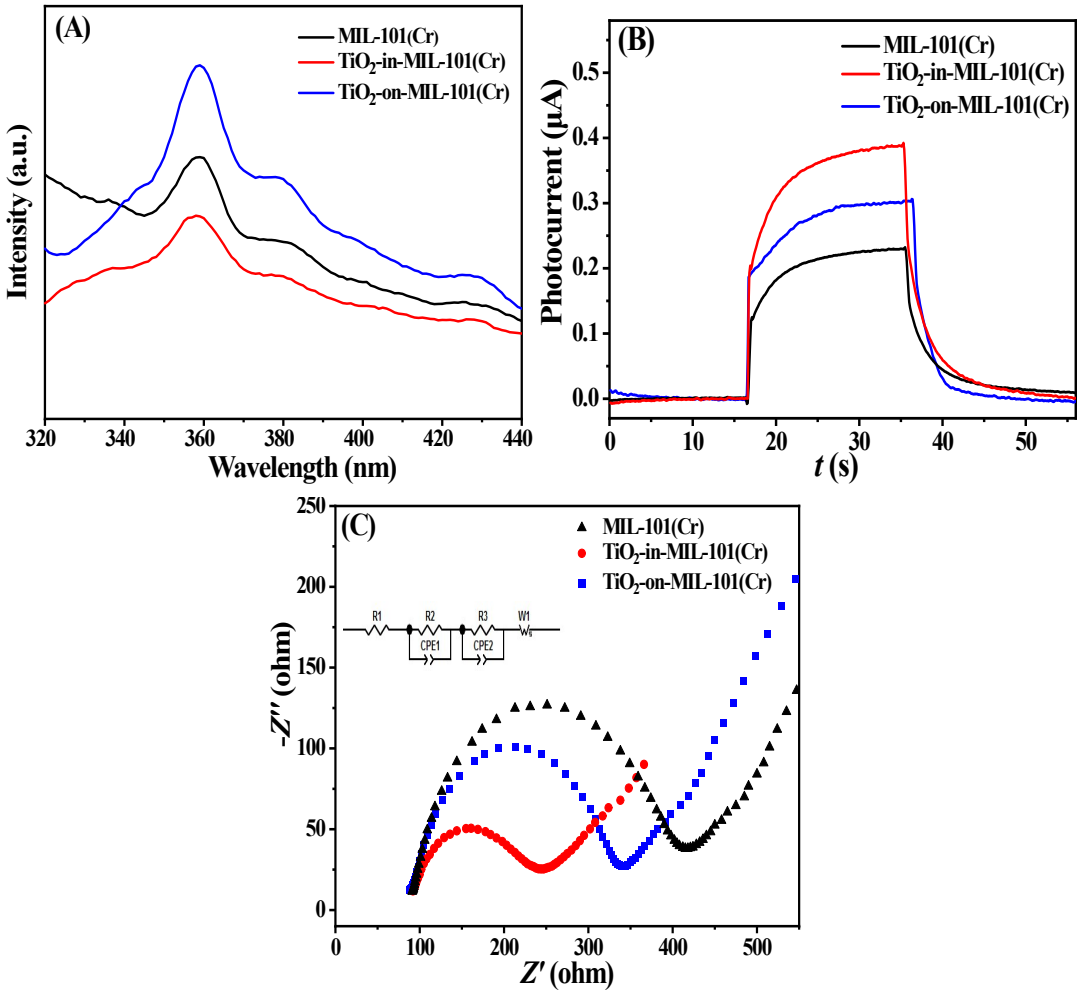


Fig. S2 (A) The fluorescence emission spectrum, (B) Photocurrent curves of MOFs and (C) Nyquist curves (inset is equivalent circuit diagram).

3. The kinetic process of MO adsorption and photocatalytic decolorization

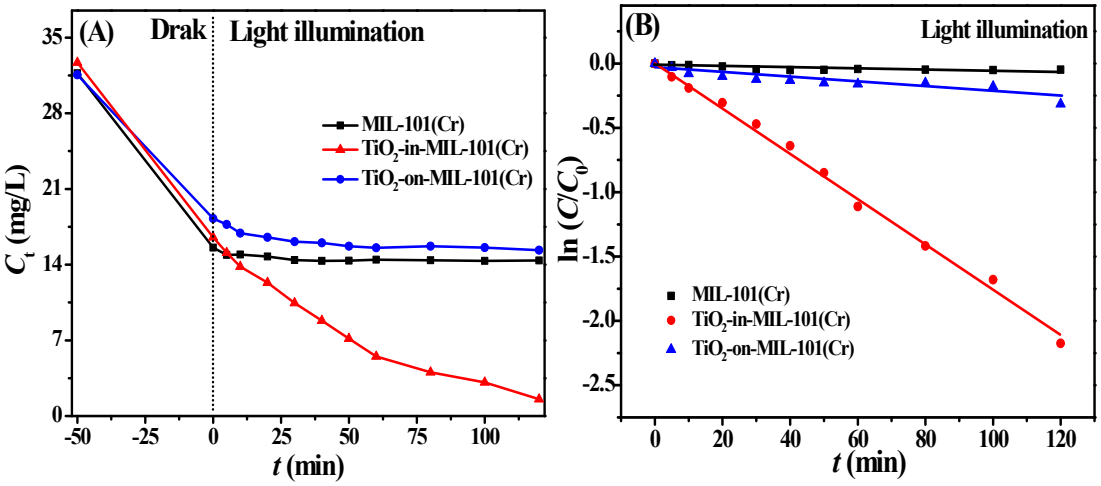


Fig. S3 (A) Adsorption and photocatalytic decolorization kinetics of MO in dark and under light and (B) ln(C/C_0) as function of time.

4. EPR characterization

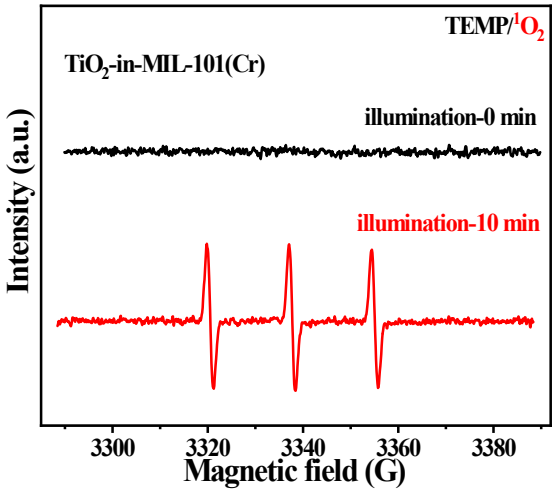
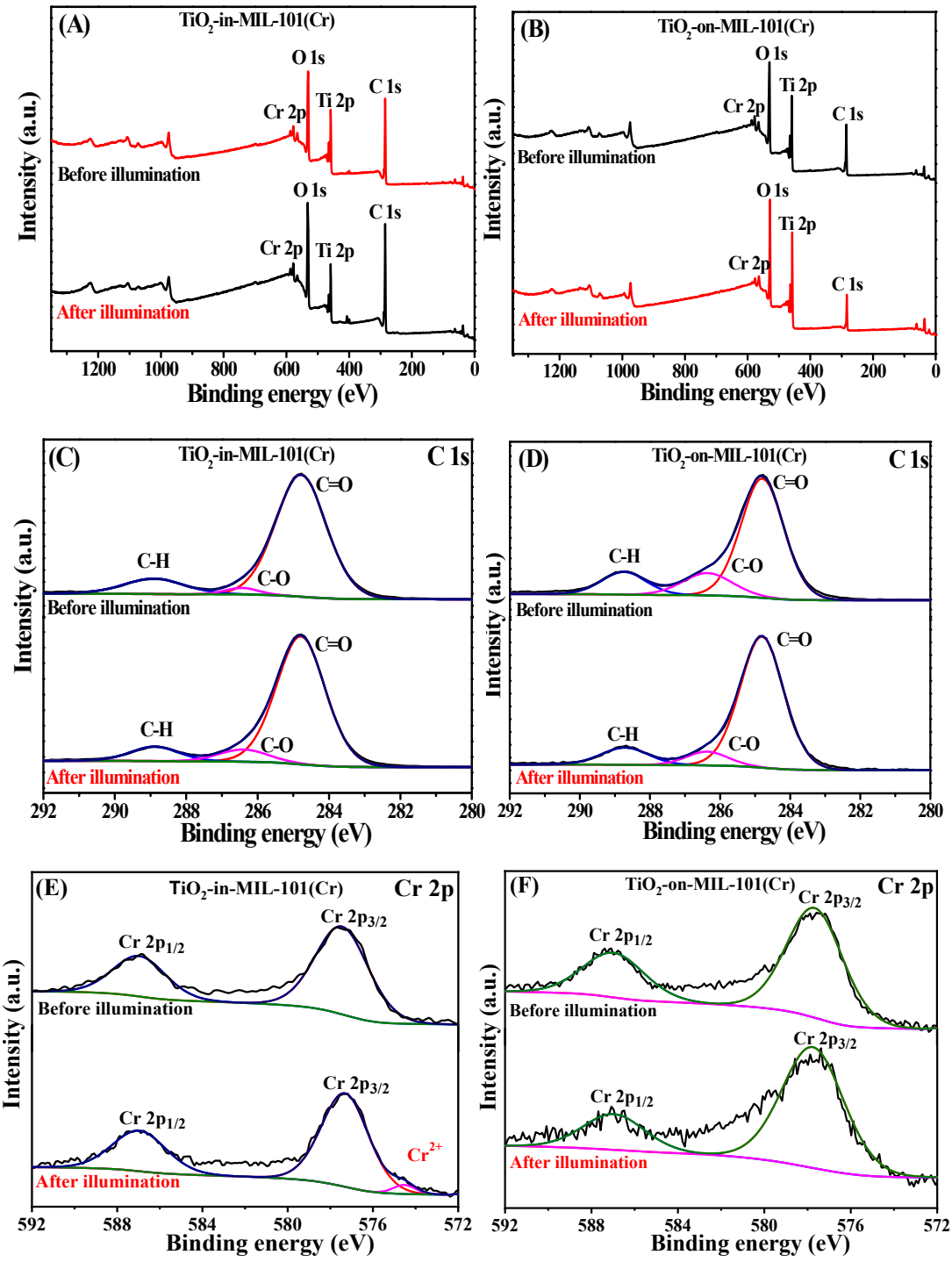


Fig. S4 EPR spectra (TEMP/$^1O_2$) of TiO_2-in-MIL-101(Cr).

5. XPS characterization

For C, the ratio of the intensity of the C-O and C=O peaks for TiO_2-on-MIL-101(Cr) is greater than that of TiO_2-in-MIL-101(Cr) before illumination (Figs. S5C and S5D), this is for TiO_2 combined with -COOH on the surface of MIL-101(Cr) to form Ti-O-C-OH bond, resulting in an increase in the content of C-O. For Cr, a new peak of 574.8 eV representing Cr^{2+} appears in TiO_2-in-MIL-101(Cr) after illumination (Fig. S5E),[1] which is not observed in TiO_2-on-MIL-101(Cr) (Fig. S5F). In addition, for the O 1s spectrum, the peaks near 533.0, 531.9 and 530.0 eV corresponds to -OH of H_2O, O-C=O and Ti-O, respectively.[2,3] The ratio of the peak intensity of O-C=O to that of Ti-O for TiO_2-in-MIL-101(Cr) (Fig. S5H) is significantly greater than that for TiO_2-on-MIL-101(Cr) (Fig. S5G) before illumination. It can be interpreted that TiO_2 of TiO_2-in-MIL-101(Cr) combines with Cr to form Ti-O-Cr bond, which has almost no effect on -COOH. However, for TiO_2-on-MIL-101(Cr), TiO_2 combines with -COOH on the surface of MIL-101(Cr) to form Ti-O-C-OH bond, which leads to the reduction of -COOH, which is in accordance with the results of DFT calculations. Furthermore, the intensity ratios of O-C=O to Ti-O peaks reduce after illumination, which may be attributed to the adsorption of O_2 on the surface TiO_2 that lead to the formation of Ti-O bond. The binding energy peaks at 458.6 eV and 464.5 eV corresponds to Ti^{4+} of TiO_2.[4] The XPS peaks of Ti for TiO_2-in-MIL-101(Cr) and TiO_2-on-MIL-101(Cr) did not change significantly after illumination, indicating that

the photocatalytic reaction has no effect on the oxidation state of Ti (Figs. S5I and S5J).



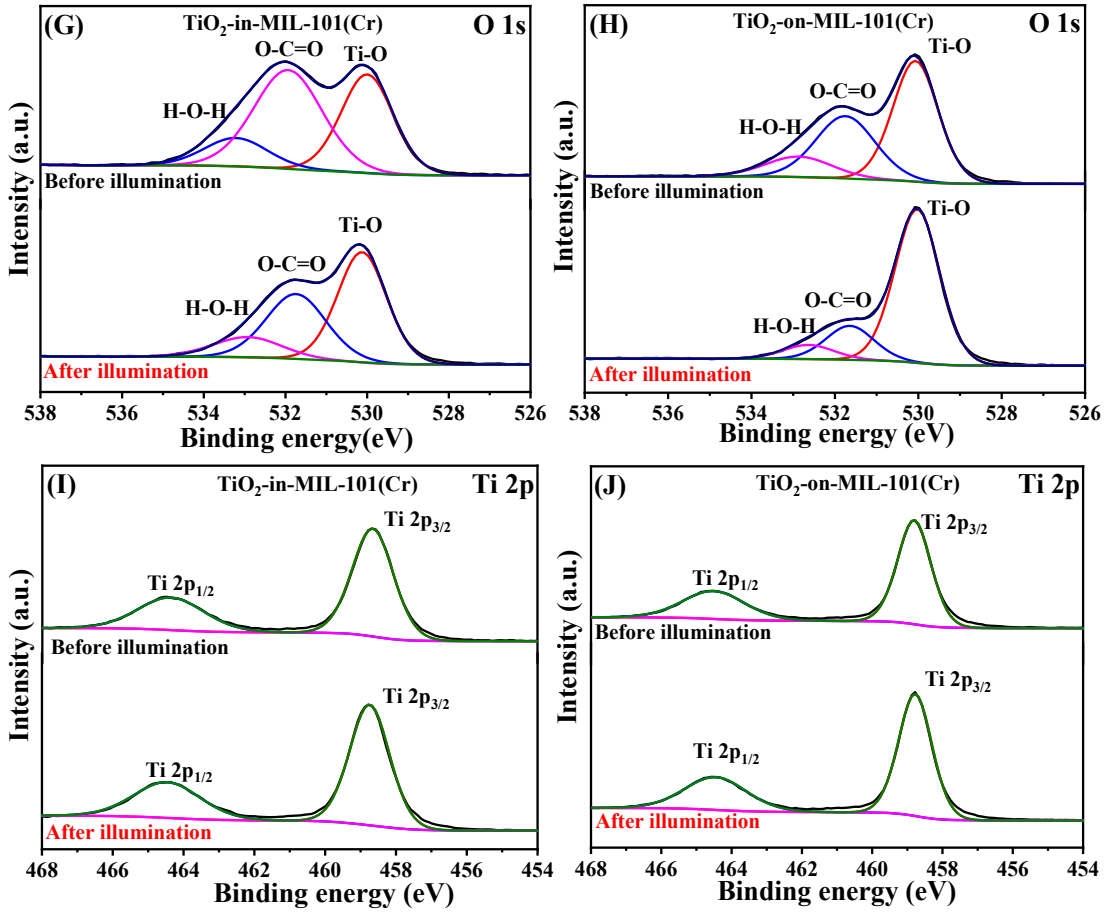


Fig. S5 (A-J) XPS spectra of TiO_2-in-MIL-101(Cr) and TiO_2-on-MIL-101(Cr) before and after illumination.

6. Results from DFT calculations

Table S1 Binding energy of TiO_2 and MIL-101(Cr) in the aqueous and alcoholic phases

Binding sites	Aqueous phase		Alcoholic phases	
	***E*(eV)**	***E*$_b$ (eV)**	***E* (eV)**	***E*$_b$ (eV)**
Ti-O-Cr	-4589.50	1.83	-4589.55	3.60
Ti-O-C-OH	-4589.52	2.51	-4589.46	1.09

Table S2 NPA charges of TiO_2 in the aqueous and alcoholic phases

Sample	Aqueous phase		Alcoholic phases	
	Excited state (|e|)	**Ground state (|e|)**	**Excited state (|e|)**	**Ground state (|e|)**
TiO_2-in-MIL-101(Cr)	-0.184	-0.225	-0.313	-0.742
TiO_2-on-MIL-101(Cr)	-0.277	-0.277	-0.282	-0.283

References

1 R. Hossain, A. Billah, M. Ishizaki, S. Kubota, F. Hirose and B. Ahmmad, Oxygen vacancy mediated room-temperature ferromagnetism and band gap narrowing in $DyFe_{0.5}Cr_{0.5}O_3$ nanoparticles, *Dalton Trans.*, 2021, 50, 9519-9528.

2 Z. L. Cheng, L. Gan, X. Chu, D. W. Wang, Z. M. Qi, J. Jiang and T. J. Zhang, Investigation of the microwave dielectric properties of the $Li_4x/_3Zn_2-_2xTi_{1+2x/3}O_4$ system by P–V–L theory and vibration spectroscopy, *Ceram. Int.*, 2021, 47, 34695-34703.

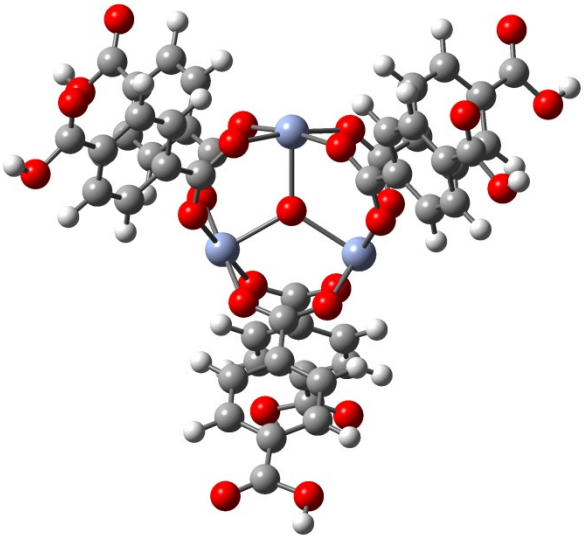
3 J. F. Chen, X. D. Zhang, X. Y. Shi, F. K. Bi, Y. Yang and Y. X. Wang, Synergistic effects of octahedral TiO_2-MIL-101(Cr) with two heterojunctions for enhancing visible-light photocatalytic degradation of liquid tetracycline and gaseous toluene, *J. Colloid Interface Sci.*, 2020, 579, 37-49.

4 W. Wu, T. T. Yao, Y. Xiang, H. Zou, Y. Zhou, Efficient removal of methyl orange by a flower-like TiO_2/MIL-101(Cr) composite nanomaterial. *Dalton Trans.*, 2020, 49, 5722-2729.

Appendix

Optimized structures and Cartesian coordinates

1. Water solvent



MOF

Energies = -3965.701237 a.u

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Cr	-1	-0.00137400	-0.02623100	2.35184300
Cr	-1	-0.01051100	-1.85580600	-1.00157200

C	0	-1.80845400	0.04257300	-2.57340900
O	0	-1.36741600	-1.11353000	-2.21343600
O	0	-1.35845100	1.18983600	-2.19790600
C	0	1.80847900	0.02323100	-2.57250100
O	0	1.36877800	1.17472100	-2.19766900
O	0	1.35792000	-1.12860600	-2.21080600
C	0	-1.80904300	2.34658900	1.40169800
O	0	-1.34131600	2.60636600	0.21522600
O	0	-1.38476100	1.46707800	2.22284700
C	0	1.84039400	2.31825700	1.39860600
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O	0	1.34284400	-2.58160600	0.17893400
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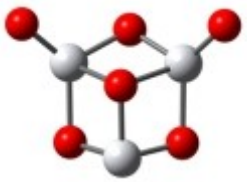

$(TiO_2)_3$

Energies = -623.730625 a.u

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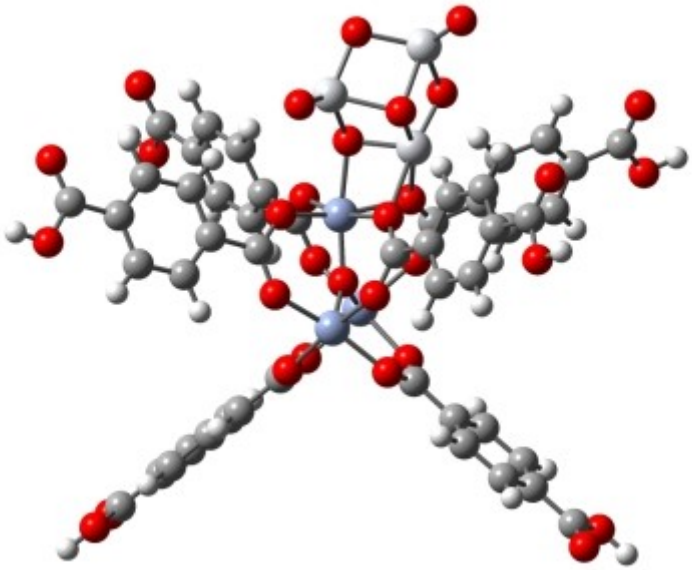
O	1.39736500	1.31570900	-0.61796500
O	-0.00017800	0.10951300	0.99716900
Ti	1.42278600	-0.60554600	-0.19958100
Ti	-1.42345200	-0.60456700	-0.19950000
O	2.52006100	-1.44456600	0.70996300
O	-0.00070600	-1.53426500	-0.91090600
O	-2.52096300	-1.44298300	0.71022400



MOF-$(TiO_2)_3$-C

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Cr	0	-0.75195600	1.28928500	-1.76267900
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C	-1	1.45042400	5.80732900	0.39924500
C	-1	1.52556400	5.39193400	-1.99532500
C	-1	2.16206900	6.98826800	0.21953200
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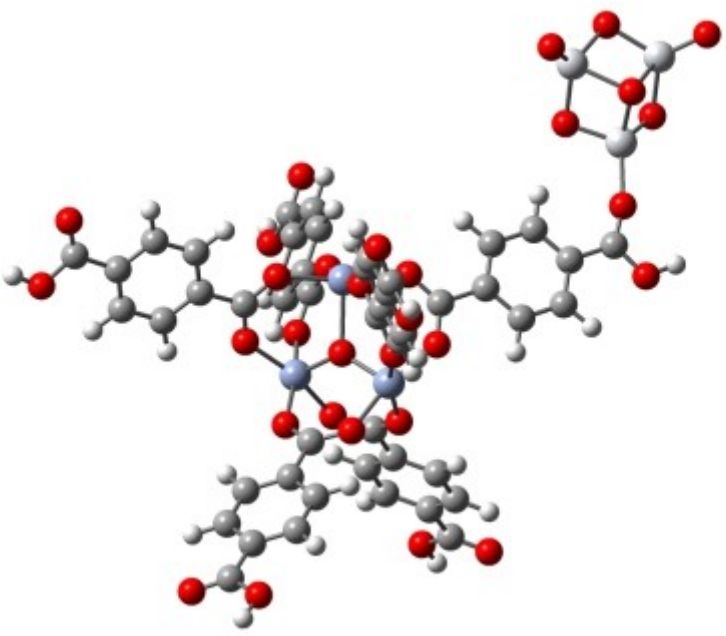
C	-1	2.23691500	6.57124600	-2.17345500
H	-1	1.26820000	4.76000000	-2.83594900
C	-1	2.55398400	7.36733300	-1.06834000
H	-1	2.41760900	7.61843300	1.06124000
H	-1	2.55617700	6.89422100	-3.15748100
C	-1	-8.42814300	4.50028700	-0.83161400
O	-1	-9.08169900	4.89476400	0.13348900
O	-1	-8.91134100	4.48376800	-2.11038500
H	-1	-9.84318400	4.82967400	-2.12580800
C	-1	3.31357100	8.61302600	-1.32083700
O	-1	3.68817400	8.99754900	-2.42807400
O	-1	3.55681200	9.30058300	-0.16451900
H	-1	4.06722200	10.13006300	-0.36380000
C	-1	6.60902600	-0.93583000	-5.20260500
O	-1	7.47773600	-1.76153600	-4.92297100
O	-1	6.70343300	-0.07730200	-6.26302300
H	-1	7.55807500	-0.23003300	-6.74722500
C	-1	-5.28251500	-5.08785900	-4.78786100
O	-1	-5.43181100	-6.26763400	-4.47087900
O	-1	-5.95472300	-4.49814300	-5.82268200
H	-1	-6.55731700	-5.15962600	-6.25571800
C	-1	-5.53742900	-3.27714800	6.12487300
O	-1	-5.67873500	-4.49779100	6.19352200
O	-1	-6.25349000	-2.39512400	6.88632000
H	-1	-6.87914300	-2.89026200	7.47930000
C	-1	6.36381400	0.92596900	5.68635500
O	-1	7.24400800	0.06635900	5.71752900
O	-1	6.41486200	2.07883100	6.42041900
H	-1	7.24939700	2.09971700	6.96018700
Ti	0	2.53185400	-2.14917500	0.58587600
O	0	3.48536300	-3.03935700	1.74051000
O	0	0.88888800	-2.87449900	0.61034000
O	0	2.94641600	-3.54459200	-0.59927700
Ti	0	1.24495900	-4.54182600	-0.47952200
Ti	0	3.81619500	-4.70929600	0.73079400
O	0	0.83421200	-4.97317500	-2.01740800
O	0	2.30811000	-5.73194500	0.42934600

O	0	5.25446100	-5.24248000	0.11831600



MOF-$(TiO_2)_3$-S

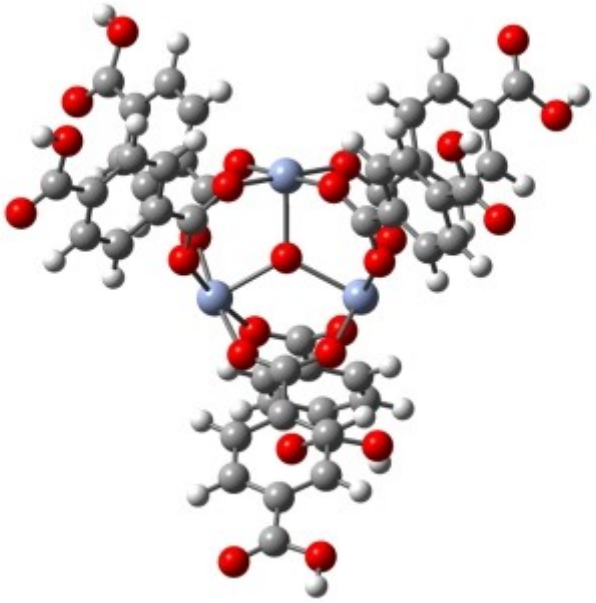
Energies = -4589.524209 a.u

O	0	-1.95233400	0.33103800	-0.08942000
Cr	0	-1.74453900	0.09275200	-1.87275900
Cr	0	-0.71006000	-0.95212500	1.19778700
Cr	0	-2.97575500	1.55513900	0.77076200
C	-1	-1.93761100	3.04142200	-1.59350700
O	-1	-2.49961700	3.03829900	-0.43384800
O	-1	-1.63224900	2.01127800	-2.30433400
C	-1	-4.62915400	0.62666000	-1.50926900
O	-1	-3.66216700	0.19100700	-2.24064300
O	-1	-4.52678700	1.21784700	-0.36884200
C	0	1.13178200	-0.30397500	-1.10412400
O	0	0.18784200	0.00741900	-1.93275500
O	0	0.95436400	-0.69792500	0.09641100
C	-1	-1.58720400	-2.78015800	-1.08738700
C	-1	-3.33751500	-0.68843400	2.71534500
C	0	-0.58682800	1.73567300	2.56898700
O	-1	-2.23055000	-1.28595200	2.49804800
O	-1	-3.73556100	0.43548700	2.19712100
O	0	-0.11883200	0.56417100	2.36350800
O	0	-1.66513100	2.20187400	2.01876600
O	-1	-1.79359200	-1.87529300	-1.99988500
O	-1	-1.13525100	-2.59813300	0.09172800
C	0	0.13994100	2.63842400	3.49900400
C	0	-0.34721800	3.92628800	3.74946400
C	0	1.31156000	2.18579300	4.11741800
C	0	0.33784800	4.76600700	4.62076600
H	0	-1.25577100	4.25310000	3.25917500
C	0	1.99488900	3.02567200	4.98660600
H	0	1.66744000	1.18476700	3.90738900
C	0	1.50860700	4.31284300	5.23722100
H	0	-0.02093000	5.76540200	4.82894700
H	0	2.90485100	2.70653700	5.48122800
C	-1	-4.29170600	-1.32975400	3.67101200
C	-1	-3.94188900	-2.54140900	4.27811600
C	-1	-5.51987300	-0.72202500	3.95379000
C	-1	-4.82246800	-3.14306400	5.16745400
H	-1	-2.98539500	-2.99145800	4.04313400
C	-1	-6.40136600	-1.32448600	4.84500800
H	-1	-5.76794700	0.21515800	3.47173100
C	-1	-6.04991300	-2.53528300	5.45045200

H	-1	-4.58093200	-4.08116200	5.65360300
H	-1	-7.35590100	-0.87066500	5.07730100
C	-1	-1.91685900	-4.18201800	-1.49143900
C	-1	-1.72244600	-5.22165900	-0.57472600
C	-1	-2.41365000	-4.44803700	-2.77209200
C	-1	-2.02614300	-6.52616100	-0.94134000
H	-1	-1.33624000	-4.99004600	0.41010200
C	-1	-2.71705300	-5.75472600	-3.13939400
H	-1	-2.55555700	-3.62713800	-3.46359800
C	-1	-2.52236100	-6.79201900	-2.22165600
H	-1	-1.88686400	-7.35276000	-0.25426100
H	-1	-3.10202300	-5.98143600	-4.12505100
C	0	2.52802500	-0.18802700	-1.61593100
C	0	3.59878000	-0.47814000	-0.76408800
C	0	2.74896900	0.20852200	-2.93906100
C	0	4.90180700	-0.37248100	-1.23263800
H	0	3.39591500	-0.78172200	0.25516700
C	0	4.04710500	0.31301200	-3.41622300
H	0	1.90178500	0.42807500	-3.57567000
C	0	5.12236200	0.02217800	-2.56195600
H	0	5.73639000	-0.58792200	-0.57420900
H	0	4.23841400	0.61656400	-4.43721700
C	-1	-1.61225800	4.37579400	-2.17498200
C	-1	-1.92118000	5.53778800	-1.45890600
C	-1	-1.00021400	4.45472200	-3.43147400
C	-1	-1.61815800	6.78318700	-1.99783800
H	-1	-2.39507300	5.45003500	-0.48931600
C	-1	-0.69766600	5.69916900	-3.96851100
H	-1	-0.77108200	3.54218200	-3.96721600
C	-1	-1.00617600	6.86039600	-3.25296600
H	-1	-1.84838400	7.69377100	-1.46053300
H	-1	-0.22338500	5.79492500	-4.93829000
C	-1	-6.00955600	0.43161400	-2.03932600
C	-1	-6.19492700	-0.19724000	-3.27567700
C	-1	-7.10797300	0.87888600	-1.29566000
C	-1	-7.48066300	-0.38082000	-3.77220100
H	-1	-5.32901400	-0.53376200	-3.83187200
C	-1	-8.39165200	0.69430600	-1.79227600
H	-1	-6.94003000	1.36316900	-0.34198700
C	-1	-8.57704500	0.06608600	-3.02780600
H	-1	-7.64588400	-0.86463500	-4.72588200
H	-1	-9.26305400	1.02818400	-1.24116000
C	-1	-0.65974600	8.15802000	-3.87637900
O	-1	-0.12032700	8.29055100	-4.97439300
O	-1	-1.01361300	9.21191500	-3.08070900
H	-1	-0.76928800	10.06817300	-3.52269300
C	-1	-9.96854900	-0.10213900	-3.50519300
O	-1	-10.97188100	0.26643800	-2.89557500
O	-1	-10.01448500	-0.72464000	-4.72147900
H	-1	-10.95862100	-0.82423900	-5.01636400
C	-1	-6.94686500	-3.22199200	6.40665600
O	-1	-6.69547400	-4.28718300	6.96951900
O	-1	-8.10936300	-2.52772800	6.59916900
H	-1	-8.68993900	-3.01193500	7.24466500
C	0	2.27995600	5.16293000	6.17256000
O	0	3.31498600	4.82210000	6.74413300
O	0	1.70269400	6.39176700	6.33276200
H	0	2.24072700	6.93974000	6.96389600
C	0	6.48670800	0.13034600	-3.06217900
O	0	7.51713300	-0.11376500	-2.36755500
O	0	6.60466800	0.50962100	-4.32794600
H	0	7.55359000	0.56936500	-4.62891900
C	-1	-2.82702800	-8.20111800	-2.55610600
O	-1	-2.67872800	-9.15529600	-1.79308900
O	-1	-3.30033100	-8.32820600	-3.83297000
H	-1	-3.49403100	-9.28341900	-4.02862900
Ti	0	8.80989000	-0.55748000	-0.94936200
O	0	10.41481800	0.12305300	-0.68138600
O	0	8.00452600	-0.65853400	0.60889000
O	0	9.56304200	-2.19860700	-0.53936700
Ti	0	8.90860300	-2.24399500	1.33381700

Ti	0	11.31893000	-1.44424900	0.04045400
O	0	8.22742100	-3.72393700	1.62503900
O	0	10.69842300	-1.98984200	1.69340900
O	0	12.53596200	-2.29042300	-0.69752400

2. Ethanol solvent



MOF

Energies = -3965.697229 a.u

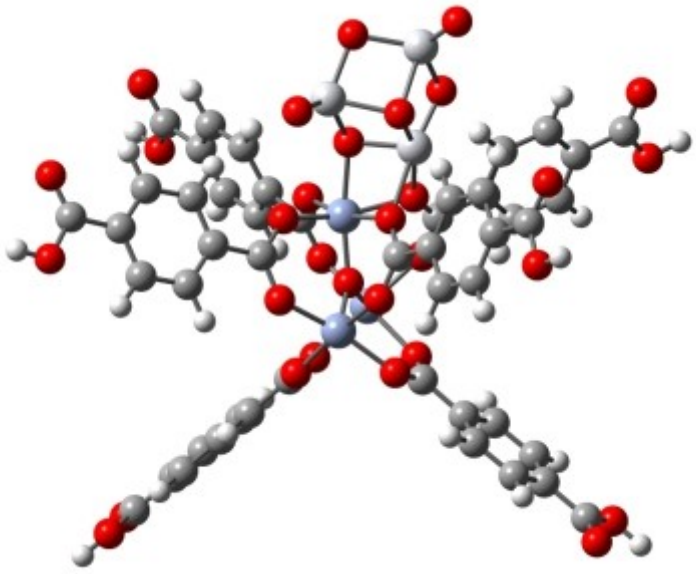
O	-1	0.00003800	-0.01686400	0.15049500
Cr	-1	-0.01007200	-1.89556300	-0.99422500
Cr	-1	0.00040100	0.01027000	2.35032700
Cr	-1	0.00993500	1.86479900	-0.98935100
C	0	1.80830800	-0.02394400	-2.57455000
O	0	1.36547300	1.12913200	-2.20763200
O	0	1.35916200	-1.17489800	-2.20804300
C	0	-1.80775400	-0.00516100	-2.57559200
O	0	-1.36495500	-1.15988500	-2.21349800
O	0	-1.35823100	1.14395100	-2.20437700
C	0	1.80136900	-2.35873900	1.38875500
O	0	1.33720100	-2.60640400	0.19832700
O	0	1.37481100	-1.48770200	2.21803800
C	0	-1.84445400	-2.32089000	1.37945500
C	0	-1.80508800	2.35801000	1.38820200
C	0	1.84745800	2.32177600	1.37798300
O	0	-1.37726100	1.49728800	2.22842100
O	0	-1.34088800	2.58583300	0.19500500
O	0	1.41334200	1.46446400	2.21839000
O	0	1.37443600	2.56586000	0.19129600
O	0	-1.37308700	-2.58287600	0.19482300
O	0	-1.40984700	-1.45514100	2.20994200
C	0	3.02243500	3.15189500	1.78473900
C	0	3.54407800	4.11098300	0.90973300
C	0	3.59142100	2.95937900	3.04892100
C	0	4.63564100	4.88070500	1.29722200
H	0	3.08714000	4.24092300	-0.06314200
C	0	4.68160200	3.72764500	3.43546200
H	0	3.16935000	2.21071400	3.70765800
C	0	5.20232800	4.68696600	2.56108500
H	0	5.05398800	5.62787600	0.63555500
H	0	5.14460400	3.60261900	4.40742300
C	0	-2.95960400	3.21218100	1.80319100
C	0	-3.52024900	3.03495600	3.07333100
C	0	-3.47087600	4.17816400	0.92964400

C	0	-4.59185600	3.82530800	3.46719800
H	0	-3.10663300	2.28042100	3.73073300
C	0	-4.54365600	4.97017000	1.32459200
H	0	-3.02075600	4.29596800	-0.04795000
C	0	-5.10218100	4.79153900	2.59429300
H	0	-5.04821700	3.71239700	4.44377400
H	0	-4.95374600	5.72299100	0.66417600
C	0	-3.02163500	-3.14456700	1.79548900
C	0	-3.59045400	-2.93612000	3.05718400
C	0	-3.54562000	-4.11232400	0.93153600
C	0	-4.68285500	-3.69688200	3.45224800
H	0	-3.16643300	-2.18112800	3.70741300
C	0	-4.63946600	-4.87453100	1.32746400
H	0	-3.08866200	-4.25476200	-0.03956000
C	0	-5.20610900	-4.66468400	2.58877200
H	0	-5.14564200	-3.55948400	4.42265600
H	0	-5.05961000	-5.62813600	0.67426700
C	0	2.95804500	-3.20644300	1.81347100
C	0	3.51826500	-3.01337900	3.08145900
C	0	3.47187000	-4.18105500	0.95109500
C	0	4.59194500	-3.79634100	3.48434400
H	0	3.10252400	-2.25262100	3.73030800
C	0	4.54703900	-4.96539700	1.35484100
H	0	3.02197200	-4.31124800	-0.02501400
C	0	5.10513700	-4.77086200	2.62239300
H	0	5.04778800	-3.67119800	4.45968500
H	0	4.95925000	-5.72443000	0.70289100
C	0	2.95509300	-0.02715100	-3.52830800
C	0	3.49119300	1.18708200	-3.97166900
C	0	3.48575800	-1.24420000	-3.97168300
C	0	4.56058400	1.18755200	-4.86024200
H	0	3.06301800	2.11486700	-3.61360300
C	0	4.55399100	-1.24255800	-4.85896800
H	0	3.05463700	-2.17097700	-3.61480400
C	0	5.08973200	-0.02922600	-5.30203700
H	0	4.99032300	2.11518200	-5.21478300
H	0	4.98862800	-2.16710500	-5.22075900
C	0	-2.95454400	0.00199900	-3.52925800
C	0	-3.49100500	-1.21025300	-3.97744600
C	0	-3.48484500	1.22099900	-3.96778400
C	0	-4.56038000	-1.20681800	-4.86602400
H	0	-3.06316700	-2.13962100	-3.62311700
C	0	-4.55303700	1.22326200	-4.85513700
H	0	-3.05334800	2.14617300	-3.60719500
C	0	-5.08911600	0.01186900	-5.30305600
H	0	-4.99036900	-2.13287600	-5.22434700
H	0	-4.98728700	2.14942000	-5.21324600
C	0	6.22799100	-0.09106200	-6.24675600
O	0	6.73769700	-1.12804400	-6.66962600
O	0	6.65717400	1.15709900	-6.60448300
H	0	7.42060300	1.08417200	-7.23695400
C	0	-6.22711100	0.07764100	-6.24783900
O	0	-6.73635100	1.11634400	-6.66700400
O	0	-6.65718100	-1.16902300	-6.60971300
H	0	-7.42067500	-1.09350000	-7.24179400
C	0	-6.24366100	5.60478900	3.06921600
O	0	-6.77865900	5.49446800	4.17194700
O	0	-6.64674800	6.51167400	2.12759600
H	0	-7.41271000	7.04135300	2.47527700
C	0	6.36322500	5.47686600	3.02824600
O	0	6.90551800	5.35330200	4.12599500
O	0	6.77559100	6.37835200	2.08542400
H	0	7.55419200	6.89270600	2.42800800
C	0	6.24901300	-5.57529300	3.10630900
O	0	6.78316600	-5.45175300	4.20805500
O	0	6.65559600	-6.49073500	2.17445800
H	0	7.42308400	-7.01416300	2.52817400
C	0	-6.36952100	-5.44569100	3.06436700
O	0	-6.91165300	-5.30846600	4.16058500
O	0	-6.78395800	-6.35701600	2.13190300
H	0	-7.56394300	-6.86534000	2.48027300

$(TiO_2)_3$

Energies = -623.724729 a.u

Ti	0.00027100	1.81917900	0.29849600
O	-1.39741800	1.31669600	-0.61859700
O	1.39867700	1.31579100	-0.61762900
O	-0.00049300	0.11297300	1.00077900
Ti	1.42309900	-0.60589000	-0.19625700
Ti	-1.42371900	-0.60555400	-0.19660900
O	2.52909900	-1.44300300	0.70235600
O	-0.00035500	-1.53118400	-0.91082800
O	-2.52855000	-1.44254300	0.70343500



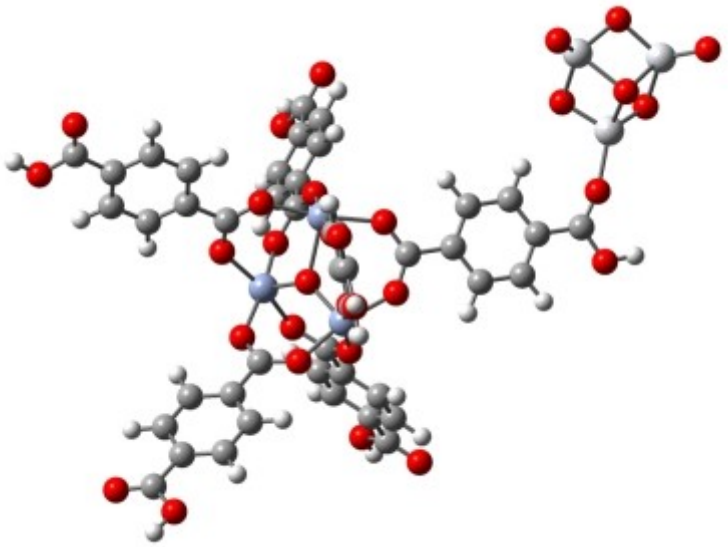
MOF-$(TiO_2)_3$-C

Energies = -4589.554264 a.u

O	0	-0.55081500	0.71204000	-0.01049400
Cr	0	-0.85810800	1.79459100	1.46477300
Cr	0	0.07143800	-1.13410000	0.26458400
Cr	0	-0.78044000	1.35248400	-1.74110700
C	0	-3.10107800	2.53180300	-0.31180400
O	0	-2.50479600	2.14851100	-1.38945800
O	0	-2.54687000	2.49204800	0.85468700
C	0	0.35503200	3.76296300	-0.40895900
O	0	0.04366900	3.37461400	0.78244000
O	0	0.08161000	3.06525600	-1.46095400
C	0	-1.85753200	-0.79955100	2.51166800
O	0	-1.82312700	0.49066700	2.51826300
O	0	-1.16270500	-1.52000200	1.69778200
C	0	1.68925100	0.45072800	2.37891100
C	0	1.77853000	-0.17332200	-2.16179000
C	0	-1.77033100	-1.43989400	-2.06628300
O	0	1.66141000	-0.88569700	-1.06786800
O	0	0.88667900	0.67924000	-2.50273700
O	0	-1.13562500	-1.90404600	-1.04199000
O	0	-1.68694500	-0.20945900	-2.44776600
O	0	0.76806700	1.33693700	2.44512800

O	0	1.61924100	-0.54815300	1.52587400
C	-1	-2.64667900	-2.36404200	-2.82750000
C	-1	-3.40976600	-1.86102400	-3.88687100
C	-1	-2.75447300	-3.70731000	-2.44938100
C	-1	-4.28201700	-2.70046000	-4.57145600
H	-1	-3.30939400	-0.81826000	-4.16024200
C	-1	-3.62578900	-4.54519100	-3.13268500
H	-1	-2.15313200	-4.07229500	-1.62612400
C	-1	-4.38779400	-4.04247700	-4.19222000
H	-1	-4.88090100	-2.33127100	-5.39372000
H	-1	-3.73203800	-5.58985600	-2.86417400
C	-1	2.98097100	-0.34340200	-3.01549500
C	-1	3.93683600	-1.30793600	-2.67640200
C	-1	3.18892100	0.51060700	-4.10408700
C	-1	5.09947200	-1.41625100	-3.42785000
H	-1	3.75249200	-1.95670900	-1.82923700
C	-1	4.35307300	0.40146000	-4.85704800
H	-1	2.43523400	1.24917800	-4.34625300
C	-1	5.30675900	-0.56319700	-4.51657800
H	-1	5.85880600	-2.15241500	-3.19080600
H	-1	4.53302800	1.05206500	-5.70285700
C	-1	2.86479600	0.55941900	3.27605200
C	-1	3.83588000	-0.44752200	3.23193400
C	-1	3.03570100	1.67486700	4.10315400
C	-1	4.97653400	-0.33646400	4.01599200
H	-1	3.68011100	-1.30084000	2.58371400
C	-1	4.17796900	1.78581400	4.88873100
H	-1	2.27077600	2.44085800	4.11970900
C	-1	5.14691300	0.77829600	4.84322100
H	-1	5.74656300	-1.09912900	4.00420400
H	-1	4.32911900	2.64037400	5.53525200
C	-1	-2.74823200	-1.49406200	3.47061600
C	-1	-2.83606900	-2.89091100	3.46729800
C	-1	-3.55192500	-0.73410800	4.32742600
C	-1	-3.72822700	-3.52495200	4.32180400
H	-1	-2.20325400	-3.45650900	2.79480700
C	-1	-4.44522500	-1.36926900	5.18345000
H	-1	-3.46630300	0.34503800	4.31132500
C	-1	-4.53117800	-2.76518900	5.17856900
H	-1	-3.81983300	-4.60472300	4.34292900
H	-1	-5.07573600	-0.79981800	5.85372600
C	-1	-4.48464800	3.03511700	-0.41704500
C	-1	-5.10694000	3.09685000	-1.66895300
C	-1	-5.16755400	3.43317400	0.73819800
C	-1	-6.41514500	3.55699800	-1.76907000
H	-1	-4.55728200	2.78283000	-2.54735900
C	-1	-6.47420000	3.89235800	0.63707300
H	-1	-4.66566100	3.37638100	1.69581000
C	-1	-7.09608000	3.95406700	-0.61391000
H	-1	-6.91491900	3.61197200	-2.72723300
H	-1	-7.03111400	4.20718600	1.51189900
C	-1	1.06751400	5.05331100	-0.57531400
C	-1	1.38558500	5.82017900	0.55116800
C	-1	1.44881300	5.47464400	-1.85460100
C	-1	2.08668200	7.01146200	0.40132800
H	-1	1.07960400	5.47231700	1.52978200
C	-1	2.14918600	6.66454500	-2.00308500
H	-1	1.19166000	4.86459700	-2.71126700
C	-1	2.46701300	7.43091400	-0.87740800
H	-1	2.34316900	7.61900900	1.25921600
H	-1	2.45981300	7.01855600	-2.97918500
C	-1	-8.48984900	4.45142100	-0.65860500
O	-1	-9.14119300	4.81281500	0.32072900
O	-1	-8.98152500	4.46545500	-1.93458700
H	-1	-9.91678100	4.80228600	-1.93326100
C	-1	3.21505500	8.68933900	-1.09825300
O	-1	3.57831100	9.11027300	-2.19588200
O	-1	3.46173900	9.34431700	0.07658100
H	-1	3.96506800	10.18263100	-0.10242500
C	-1	6.56334900	-0.72611000	-5.28100200
O	-1	7.43973000	-1.55300200	-5.03077400

O	-1	6.64481100	0.16230300	-6.31813900
H	-1	7.49748800	0.02823600	-6.81119800
C	-1	-5.29741200	-4.98246300	-4.88423400
O	-1	-5.43513200	-6.17137700	-4.59801700
O	-1	-5.98256900	-4.37110600	-5.89835400
H	-1	-6.58305800	-5.02662600	-6.34315700
C	-1	-5.46217500	-3.49560900	6.06708900
O	-1	-5.58420300	-4.71944600	6.10901700
O	-1	-6.18726000	-2.64253300	6.85334600
H	-1	-6.80155600	-3.16184000	7.43737500
C	-1	6.38124500	0.84156900	5.65692200
O	-1	7.26879500	-0.01088200	5.66099200
O	-1	6.42735400	1.97546900	6.42105900
H	-1	7.26538400	1.98834800	6.95554100
Ti	0	2.72517800	-2.11281100	0.46160900
O	0	3.81348300	-3.04017400	1.53253400
O	0	0.92794400	-2.80682000	0.46563500
O	0	3.01628800	-3.65062500	-0.79265600
Ti	0	1.30928000	-4.48543700	-0.44982800
Ti	0	3.90210700	-4.70265800	0.57618800
O	0	0.55861800	-5.09115600	-1.80080600
O	0	2.30636400	-5.65188300	0.56859100
O	0	5.31668400	-5.39235200	0.03577500



MOF-$(TiO_2)_3$-S

Energies = -4589.461844 a.u

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Cr	0	-0.82359700	-0.76391900	1.06965000
Cr	0	-3.21899400	1.43439300	0.73420500
C	-1	-2.36412500	3.05975900	-1.60230500
O	-1	-2.91854600	2.98859800	-0.44132600
O	-1	-1.95239500	2.07330000	-2.32211700
C	-1	-4.77935400	0.36965900	-1.52296500
O	-1	-3.77511900	0.04959000	-2.26434000
O	-1	-4.73554800	0.96045200	-0.37868600
C	0	1.04196300	-0.00256500	-1.10268200
O	0	0.14003600	0.28249300	-1.95997700
O	0	0.80126500	-0.42966400	0.09809100
C	-1	-1.39154400	-2.69199400	-1.12879800
C	-1	-3.33100800	-0.81768500	2.69470700
C	0	-0.88442000	1.81669100	2.54411900
O	-1	-2.16601700	-1.28885000	2.46965700
O	-1	-3.85316000	0.25796400	2.18339600
O	0	-0.33249000	0.68047300	2.27693600

O	0	-1.98673000	2.22624900	2.02000700
O	-1	-1.69731200	-1.80921300	-2.03509700
O	-1	-0.95533800	-2.47039300	0.04964600
C	0	-0.20551100	2.70083900	3.52093700
C	0	-0.77331700	3.93946400	3.84205800
C	0	0.99544700	2.28951600	4.11193300
C	0	-0.13958500	4.77168300	4.75755200
H	0	-1.70288400	4.23401300	3.37102700
C	0	1.62643700	3.12266200	5.02603300
H	0	1.41548300	1.32707700	3.84786200
C	0	1.05980700	4.36006900	5.34730500
H	0	-0.56015100	5.73313100	5.02090200
H	0	2.55669600	2.83579700	5.50214200
C	-1	-4.20355400	-1.56377300	3.65217700
C	-1	-3.71950000	-2.73260200	4.25094000
C	-1	-5.48895700	-1.09540200	3.94539200
C	-1	-4.52299500	-3.43074100	5.14263800
H	-1	-2.72133500	-3.07445300	4.00725700
C	-1	-6.29326400	-1.79434100	4.83908700
H	-1	-5.84130100	-0.18925500	3.46902400
C	-1	-5.80747700	-2.96191100	5.43641000
H	-1	-4.17749400	-4.33906500	5.62252500
H	-1	-7.29021700	-1.44892200	5.07956600
C	-1	-1.57171500	-4.11882400	-1.53986400
C	-1	-1.26077600	-5.13676800	-0.63102700
C	-1	-2.04505400	-4.42951000	-2.81930000
C	-1	-1.42394400	-6.46423600	-1.00436300
H	-1	-0.89601300	-4.87028000	0.35311600
C	-1	-2.20804300	-5.75909000	-3.19329100
H	-1	-2.27921200	-3.62461900	-3.50446100
C	-1	-1.89648300	-6.77464900	-2.28357200
H	-1	-1.19196500	-7.27510100	-0.32360900
H	-1	-2.57263800	-6.02054700	-4.17808400
C	0	2.46902000	0.15602700	-1.48931900
C	0	3.47888200	-0.18130900	-0.58115600
C	0	2.78119000	0.63535300	-2.76671900
C	0	4.80890700	-0.04650500	-0.95283100
H	0	3.20919200	-0.54850200	0.40066400
C	0	4.10882400	0.78000100	-3.14132200
H	0	1.97857100	0.88678500	-3.44820100
C	0	5.12236600	0.43393400	-2.23338300
H	0	5.59960500	-0.30902900	-0.26069600
H	0	4.36955000	1.15044600	-4.12423300
C	-1	-2.18714000	4.42510900	-2.17613200
C	-1	-2.61500500	5.54263500	-1.45059800
C	-1	-1.59441900	4.57747400	-3.43504600
C	-1	-2.45091800	6.81677000	-1.98240200
H	-1	-3.07021600	5.39809400	-0.47888700
C	-1	-1.43080300	5.85051700	-3.96512900
H	-1	-1.27106100	3.69824100	-3.97775500
C	-1	-1.85834800	6.96726400	-3.24015500
H	-1	-2.77411400	7.69405500	-1.43762100
H	-1	-0.97495100	6.00315500	-4.93646200
C	-1	-6.13317200	0.02773400	-2.04729600
C	-1	-6.25566300	-0.61164900	-3.28600600
C	-1	-7.26980900	0.34887200	-1.29602600
C	-1	-7.51628600	-0.93215600	-3.77718000
H	-1	-5.36110400	-0.84963800	-3.84765200
C	-1	-8.52839700	0.02812900	-1.78747000
H	-1	-7.15021000	0.84338200	-0.34034900
C	-1	-8.65083100	-0.61077400	-3.02532900
H	-1	-7.63311400	-1.42710400	-4.73229600
H	-1	-9.42820000	0.26208900	-1.23051300
C	-1	-1.65676900	8.29823300	-3.85646800
O	-1	-1.14122100	8.49515700	-4.95618700
O	-1	-2.11732700	9.30351900	-3.05188100
H	-1	-1.96816900	10.18314700	-3.49025100
C	-1	-10.01801300	-0.92772700	-3.49684700
O	-1	-11.05275300	-0.67252000	-2.88194100
O	-1	-10.00202200	-1.54757200	-4.71570800
H	-1	-10.93140600	-1.74876400	-5.00539700

C	-1	-6.61718400	-3.74655600	6.39485200
O	-1	-6.24738500	-4.78011600	6.95110300
O	-1	-7.84762900	-3.18435800	6.59858800
H	-1	-8.36634400	-3.73274700	7.24538400
C	0	1.77883300	5.20464400	6.32918800
O	0	2.83510100	4.89890600	6.88068000
O	0	1.12409300	6.38267400	6.55707000
H	0	1.62683800	6.92800100	7.21883700
C	0	6.52046100	0.56217300	-2.61859600
O	0	7.48419600	0.23304000	-1.86504500
O	0	6.73945300	1.05348700	-3.83141300
H	0	7.70760800	1.11836000	-4.05965200
C	-1	-2.04877000	-8.20624700	-2.62566300
O	-1	-1.79201500	-9.14378200	-1.87098800
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H	-1	-2.60553100	-9.34573800	-4.10038100
Ti	0	8.97430700	-0.40286000	-0.74899100
O	0	10.45792400	0.53083900	-0.68209300
O	0	8.54416800	-0.82436100	0.90185600
O	0	10.05501700	-1.91158700	-0.72784800
Ti	0	9.80269200	-2.28489200	1.20576100
Ti	0	11.74209300	-0.91220300	-0.35920500
O	0	9.41914500	-3.87922300	1.42690400
O	0	11.56197900	-1.73280900	1.28243400
O	0	12.92538300	-1.41832700	-1.39874700