

Supporting Information for:
Density-functional theory models of Fe(IV)O reactivity in
metal-organic frameworks: self-interaction error, spin
delocalisation and the role of hybrid exchange

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We present here a supplementary image of Fig. 1 shown in the main text and the atomic positions and cell parameters of four Fe(IV)O-MOF74 structures including the methane molecule at the center of a MOF-74 cavity. These structures are optimised with the functionals B3LYP, BLYP, PBE, and sc-BLYP. The data are presented in “fort.34” CRYSTAL17 format, which contains information on atomic positions and crystal structures and can be visualised using the DLVisuaize software (<http://www.cse.clrc.ac.uk/cmng/DLV/>). The file format is described in the CRYSTAL17 user manual (<http://www.crystal.unito.it/Manuals/crystal17.pdf>).

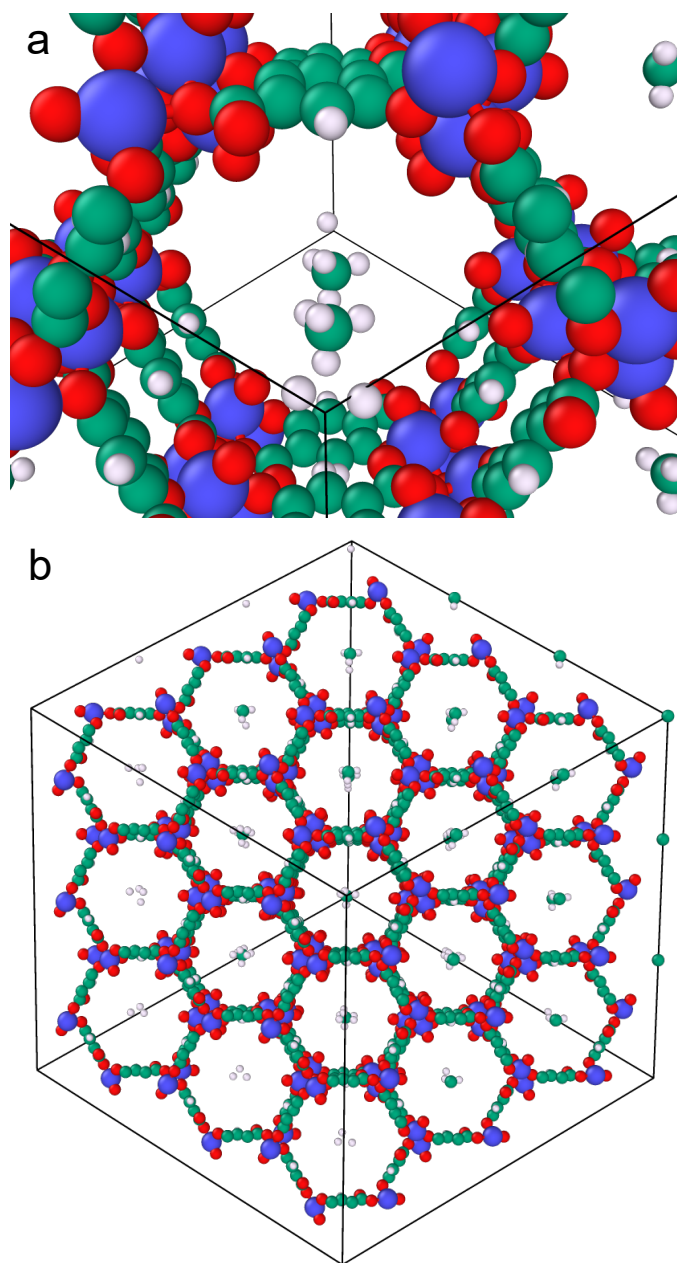


Figure S1: Zoomed (a) and general (b) views of the replicated unit cell of FeO(IV)-MOF74 by 3x3x3 times with several the methane molecules, which are separated by 6.95 Å. Atoms are painted in blue for iron, in red for oxygen, in green for carbon, and in light grey for hydrogen.

1 Coordinates for B3LYP

3 1 1 E -1.0344495038340E+04 DE-3.1E-06(6)
0.149650344474E+02 0.000000000000E+00 0.231683333333E+01
-0.748251722372E+01 0.129601000000E+02 0.231683333333E+01
-0.748251722372E+01 -0.129601000000E+02 0.231683333333E+01
1
0.100000000000E+01 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00 0.100000000000E+01 0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.100000000000E+01
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
65
26 -6.281746138992 4.047189815548 -1.331594180794
26 -0.374390795675 -7.494379612079 -1.330878344654
26 6.667496610010 3.391941440939 -1.331782140093
26 6.289767446309 -4.083134444473 1.276571676795
26 0.380640458447 7.456301822828 1.276425428334
26 -6.659043436915 -3.430361649264 1.277433129074
8 7.203919187858 3.513464122483 2.393651165359
8 -6.655182288028 4.450206638917 2.393290562885
8 -0.536990548783 -8.020320328768 2.393322066055
8 -7.195192540239 -3.551080160804 -2.448256124950
8 6.662103225554 -4.486939586097 -2.447844767379
8 0.543898036094 7.981821409464 -2.447758439987
8 6.856991645439 2.087262941712 -2.875087723921
8 -5.247074456580 4.863927873753 -2.875444137286
8 -1.598039478769 -7.006042235026 -2.875594666970
8 -6.847398102005 -2.124926134159 2.820635882835
8 5.253754767305 -4.899338804020 2.820625886850
8 1.604073001118 6.966605149699 2.821122419126
8 -7.070856788501 2.486910073589 -2.349124332868
8 1.370851635937 -7.398023254849 -2.349181154086
8 5.710998936634 4.855482648423 -2.349262555031
8 7.080470518600 -2.524119254955 2.294522771564
8 -1.364719405794 7.362105558137 2.294279331666
8 -5.704334177227 -4.894990775971 2.294877365687
6 7.127108089661 2.310132603203 2.865428649630
6 -5.575146733517 4.986280832045 2.865176404474
6 -1.540724713871 -7.352219706122 2.865163109911
6 -7.117668535753 -2.347676525036 -2.919912410734
6 5.581500111827 -5.021853165694 -2.919907944798
6 1.547208967755 7.313093244329 -2.919724615665
6 7.337071953774 1.142363729550 1.943089002062
6 -4.668709852235 5.751806324464 1.942894960089
6 -2.657456370945 -6.950583276352 1.943151961182
6 -7.326385316878 -1.179716545688 -1.997454533947
6 4.674687824490 -5.787290169991 -1.997787737348
6 2.663599118443 6.910485873193 -1.997576486678
6 -7.290187454868 1.278170711077 -1.750781881666
6 2.527545970304 -6.983889285812 -1.751013606064
6 4.773928411072 5.649844728903 -1.750892947231
6 7.300463265537 -1.315489615709 1.696309804878
6 -2.521465407638 6.948264905877 1.696084996668
6 -4.767601415312 -5.689742875167 1.696437082863
6 -7.153029696236 0.114864814725 -2.523467135977
6 3.467074368616 -6.284707005946 -2.524041152886
6 3.698618543054 6.114018692389 -2.523985991025
6 7.164542662158 -0.152213477493 2.469362940746
6 -3.461189171180 6.249394026141 2.469236779158
6 -3.692503583654 -6.154178064158 2.469599832684
1 -6.893486245798 0.227832167387 3.381070227563
1 3.239998601990 -6.117165898428 3.380218213969
1 3.667544806875 5.834265718526 3.380039656091

1 6.905466351642 -0.265273750144 -3.435051186901
1 -3.233864500559 6.081620358502 -3.435151954649
1 -3.661613002968 -5.874613962882 -3.434349231482
8 -5.073762835214 3.204049185372 -0.706593671382
8 -0.244720141361 -6.028179586951 -0.702766197675
8 5.332844801873 2.771240007884 -0.703986896076
8 5.083506540777 -3.237723021532 0.651016035628
8 0.249280825443 5.990204096531 0.648520566430
8 -5.323468022855 -2.811075539746 0.649978978569
6 0.021516865511 -0.011898252687 0.001516677787
1 0.824046467970 0.634588363080 0.370109096526
1 0.321086154722 -0.456330333616 -0.952646571258
1 -0.170524303892 -0.806665480113 0.729005160949
1 -0.888000000000 0.580000000000 -0.141000000000
0 0

2 Coordinates for BLYP

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-0.748251722372E+01 -0.129601000000E+02 0.231683333333E+01
1
0.100000000000E+01 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00 0.100000000000E+01 0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.100000000000E+01
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
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26 -0.388870918062 -7.498528935234 -1.307292363868
26 6.684670913326 3.371966185801 -1.307534169452
26 6.286388400976 -4.105036012217 1.230540267949
26 0.408475581630 7.456558072538 1.230174619536
26 -6.665020347617 -3.413991092238 1.230476997038
8 7.178820514313 3.520328727392 2.406561422833
8 -6.641433787053 4.417049804539 2.406627879770
8 -0.507960477540 -8.000059149334 2.406408163628
8 -7.158836743611 -3.562165757943 -2.483726346347
8 6.661111826950 -4.458796316535 -2.483787028188
8 0.527800860005 7.958262194694 -2.483623964417
8 6.835856042703 2.059243189180 -2.851627666899
8 -5.204393356417 4.850442109060 -2.851716361932
8 -1.601232045887 -6.971932750795 -2.851652063258
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8 1.620718446519 6.929577506499 2.774564061390
8 -7.025505509339 2.491197210815 -2.336251059997
8 1.351811068110 -7.369423722212 -2.336329809691
8 5.702785290698 4.815254477838 -2.336148887430
8 7.045434467180 -2.533015334367 2.258991056396
8 -1.332247677416 7.327846822479 2.259035832092
8 -5.683161432178 -4.857451610453 2.259046149643
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6 -4.660776941533 5.747294745529 1.952748743385
6 -2.650217727098 -6.949903534939 1.952860829487
6 -7.320615091911 -1.181712134414 -2.030030396511
6 4.680368103940 -5.788894342529 -2.030010767801
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6 4.772914775266 5.629194888362 -1.746008342061
6 7.285160102231 -1.320731918946 1.668905524440
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6 -4.753363423700 -5.671439777378 1.668891379215
6 -7.130105829119 0.121320095904 -2.543261355911
6 3.456362490637 -6.274820608827 -2.543111399203
6 3.702555434992 6.090525880372 -2.542959860845
6 7.149721969851 -0.163141173548 2.465972846756
6 -3.436824254383 6.233325700977 2.465873541003
6 -3.683278671578 -6.133203221828 2.465999292569
1 -6.855491520026 0.248707032767 3.360485904571
1 3.208286549959 -6.099522861462 3.360948638145
1 3.674966036128 5.788253681315 3.361027924617

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1 -3.189161924566 6.058881972366 -3.437920703368
1 -3.656007518887 -5.831338177063 -3.437841476080
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8 -0.260585168601 -6.016016338552 -0.638036564607
8 5.336522720954 2.741472400243 -0.638867456409
8 5.066190027658 -3.252370884726 0.562520579052
8 0.279955744374 5.974079504610 0.560948253372
8 -5.316756596892 -2.783390667224 0.562231531394
6 0.029802336887 -0.012907725367 -0.002752880927
1 0.844718719253 0.644863257708 0.338318130015
1 0.312361997603 -0.480725996047 -0.958880597773
1 -0.149325355259 -0.796942482821 0.749677888959
1 -0.888000000000 0.580000000000 -0.141000000000
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3 Coordinates for PBE

3 1 1 E -1.0342090772615E+04 DE-3.2E-06(4)
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-0.748251722372E+01 -0.129601000000E+02 0.231683333333E+01
1
0.100000000000E+01 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00 0.100000000000E+01 0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.100000000000E+01
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
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26 -6.290492188705 4.088319670163 -1.287227551039
26 -0.380609605599 -7.474093473632 -1.287249678869
26 6.677877646861 3.425647994065 -1.286754333329
26 6.294525613002 -4.063205304938 1.313695851363
26 0.387349526890 7.501991659030 1.313770276563
26 -6.674509896703 -3.396780621686 1.313259946983
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8 -6.657986150958 4.464371700032 2.434216071740
8 -0.521835602031 -7.979553540899 2.434002543284
8 -7.183613413936 -3.528609168934 -2.407929681737
8 6.663372847239 -4.438100633538 -2.407541775432
8 0.527814744015 8.008402614460 -2.407592738484
8 6.838329327884 2.110458565824 -2.821720776362
8 -5.231600592608 4.885380395234 -2.821893367973
8 -1.599917575848 -6.955418252830 -2.821801802944
8 -6.836690885675 -2.082325291666 2.848310792802
8 5.237593842309 -4.861223562594 2.848617271748
8 1.607082619557 6.985298681421 2.848414873873
8 -7.060451604724 2.520245187586 -2.302023693482
8 1.363192543607 -7.356335454164 -2.302270228342
8 5.704047984753 4.876210566276 -2.302018245971
8 7.062152217098 -2.493011124283 2.328450453115
8 -1.356568163879 7.381147757218 2.328894075676
8 -5.697947955761 -4.846182701530 2.328675951013
6 7.119182395215 2.344000945441 2.912445080596
6 -5.574267375050 5.011875889135 2.912231434638
6 -1.537983374172 -7.315160429201 2.912242657631
6 -7.117140792543 -2.316326136043 -2.885882429622
6 5.580399182616 -4.986969660437 -2.885527559390
6 1.544589441791 7.345000876159 -2.885695285607
6 7.336841356458 1.178586377548 1.993146288084
6 -4.673667262381 5.783087277462 1.993070105673
6 -2.656093922195 -6.920766608979 1.993104829516
6 -7.335471005084 -1.151208351314 -1.966494530463
6 4.680487397257 -5.758756616885 -1.966282118596
6 2.662817960744 6.951495436586 -1.966392746198
6 -7.288766159959 1.314974055232 -1.708743920049
6 2.521135624783 -6.951428395347 -1.708912617388
6 4.774775949474 5.677036721343 -1.708773105432
6 7.290139013585 -1.287721875733 1.735342337593
6 -2.514249855956 6.975751625095 1.735621178466
6 -4.768258861392 -5.646401205828 1.735489431703
6 -7.157451133801 0.147247522980 -2.489918403838
6 3.466991352782 -6.253794556932 -2.489897076556
6 3.698206168245 6.148040584634 -2.489944698653
6 7.159067771829 -0.119932143501 2.516587909849
6 -3.460283251709 6.278431622380 2.516713036252
6 -3.691311177331 -6.116947720756 2.516583480948
1 -6.889189219506 0.261483719454 3.407885595513
1 3.233975438901 -6.078187926583 3.407977628883
1 3.663140167274 5.859188638054 3.407715789947

1 6.891604554119 -0.234122178530 -3.381011229328
1 -3.227719303716 6.103835090136 -3.380910538142
1 -3.656060341008 -5.827751735720 -3.381151762608
8 -5.076948012320 3.232705408632 -0.644039770936
8 -0.248737235643 -5.995407205928 -0.643268720561
8 5.331294625997 2.800729763197 -0.642705596041
8 5.078779021744 -3.211108758089 0.670056219494
8 0.258022483046 6.023203300711 0.669727949469
8 -5.329048340246 -2.769461345752 0.669483769279
6 0.026216903136 -0.015725190479 0.001655227120
1 0.834694300049 0.634251648116 0.368980617396
1 0.324863604494 -0.465102927009 -0.957361997736
1 -0.166170263574 -0.813096104876 0.735187986060
1 -0.888000000000 0.580000000000 -0.141000000000
0 0

4 Coordinates for PBE

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-0.748251722372E+01 -0.129601000000E+02 0.231683333333E+01
1
0.100000000000E+01 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00 0.100000000000E+01 0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.100000000000E+01
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
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26 -0.375176989764 -7.487009667280 -1.325257306154
26 6.666561577164 3.380223139893 -1.326076260522
26 6.283284680850 -4.086295713441 1.255813161348
26 0.391818504829 7.445305617993 1.255501781078
26 -6.649720670500 -3.421846347160 1.256365282342
8 7.200183499442 3.512693688247 2.391564549189
8 -6.647568986579 4.440822840018 2.391463460993
8 -0.527360418915 -8.015778110343 2.391419958034
8 -7.183233986300 -3.554188484901 -2.461397536431
8 6.664227791636 -4.482348586167 -2.461377960474
8 0.544192527082 7.974172497114 -2.461278626362
8 6.842700401292 2.079939827841 -2.879559861060
8 -5.228125060484 4.847711214641 -2.879654184110
8 -1.588681741370 -6.988934633543 -2.879812178262
8 -6.825891704382 -2.121398309443 2.809719759839
8 5.244853986072 -4.889258666775 2.809642058190
8 1.605402684891 6.947117922696 2.809992095999
8 -7.053738574266 2.482596376724 -2.352075939471
8 1.371247639306 -7.388075925468 -2.352034882995
8 5.707386208456 4.843614451928 -2.352185581896
8 7.070891448751 -2.524070327912 2.282268530895
8 -1.354749050310 7.346834651302 2.282066805667
8 -5.690767547482 -4.885512506667 2.282394954465
6 7.118871481675 2.307718051145 2.861172490857
6 -5.563227460957 4.972713661566 2.861061909794
6 -1.529881652405 -7.342331059055 2.861032826878
6 -7.101934695287 -2.349222008908 -2.930995622844
6 5.579928303748 -5.014222019376 -2.931045546087
6 1.546598287411 7.300588826034 -2.930866529910
6 7.332878335766 1.140208707054 1.937789959788
6 -4.659116361276 5.741656559722 1.937587895692
6 -2.648225710706 -6.944241331532 1.937705425896
6 -7.315877800319 -1.181695441835 -2.007589710473
6 4.675751757834 -5.783140927686 -2.007583226137
6 2.664876800115 6.902369774439 -2.007509184927
6 -7.278444805405 1.274854500961 -1.754097499632
6 2.529707631227 -6.979044325110 -1.754154710109
6 4.773766467273 5.642019987523 -1.754101753570
6 7.295484916723 -1.316346421127 1.684305229822
6 -2.513032847531 6.937513683397 1.684135033260
6 -4.757131880940 -5.683861366051 1.684287130949
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6 3.463353155335 -6.273227374096 -2.530282188821
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6 7.151421878750 -0.154837266042 2.460545051045
6 -3.446654417986 6.231622223822 2.460249812969
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8 -0.245804999513 -6.019707345501 -0.683883799753
8 5.331131737520 2.758552461003 -0.684778696745
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8 0.262266312970 5.977951972749 0.614323559184
8 -5.314107003198 -2.800275252565 0.615434227816
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1 0.825916199824 0.636309783342 0.367842739612
1 0.321613581622 -0.456129948749 -0.954735787633
1 -0.167479475198 -0.806735559071 0.728820809305
1 -0.888000000000 0.580000000000 -0.141000000000
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