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Supporting information for article:

Band-gap assessment from X-ray powder diffraction using Artificial Intelligence

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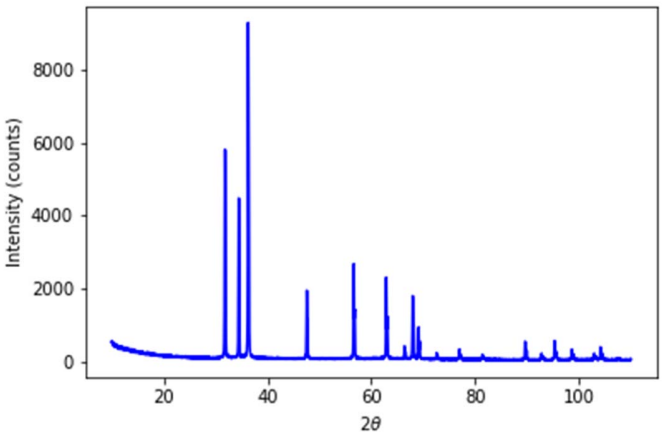
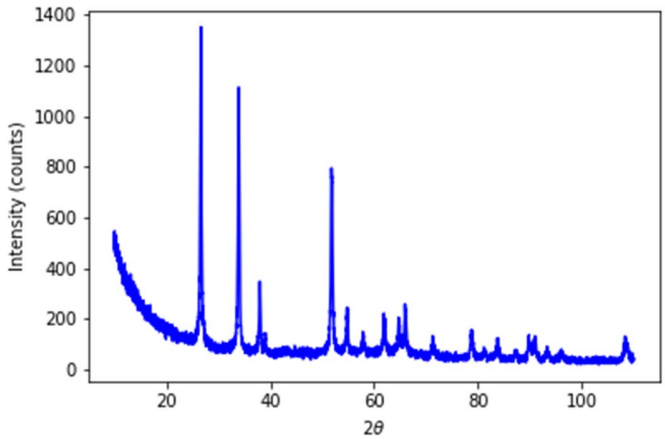
A. Recorded diffraction patterns

a) ZnO

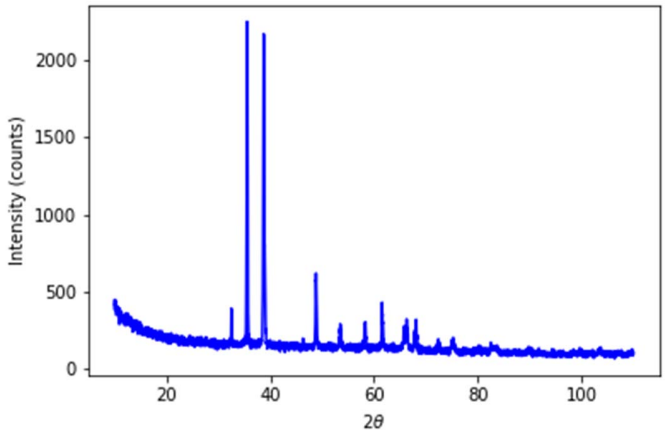


b) SnO_2



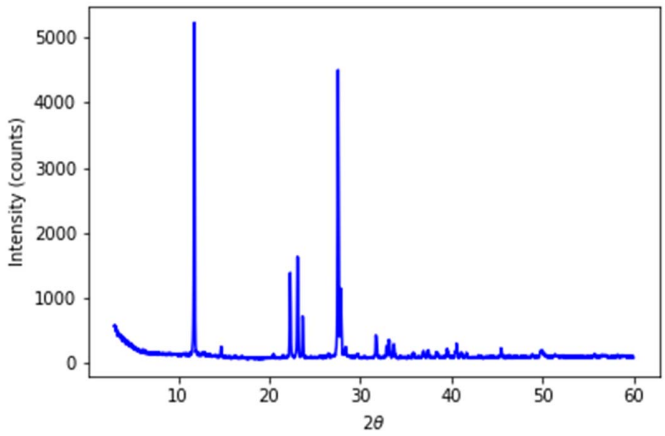
The background noise before the first peak was removed up to 2θ=20°

c) CuO

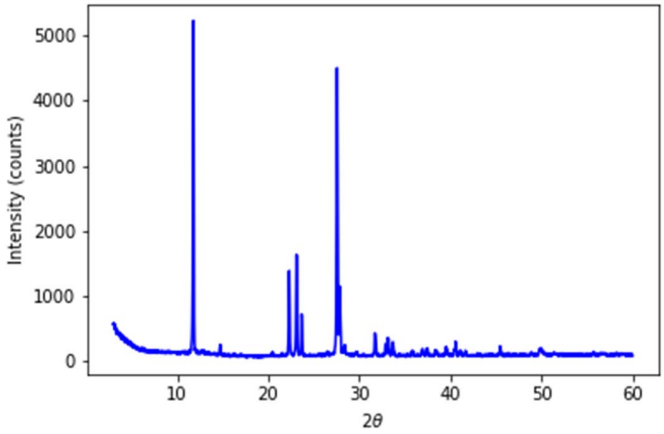


After Rietveld refinement, it was assessed that the actual crystal size of the sample was 107 nm.

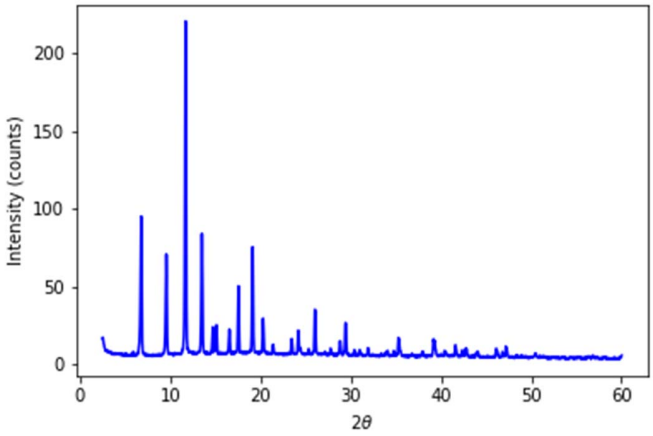
d) 1, 4, 5, 8-Naphtalenetetracarboxilic dianhydride, NTCDA



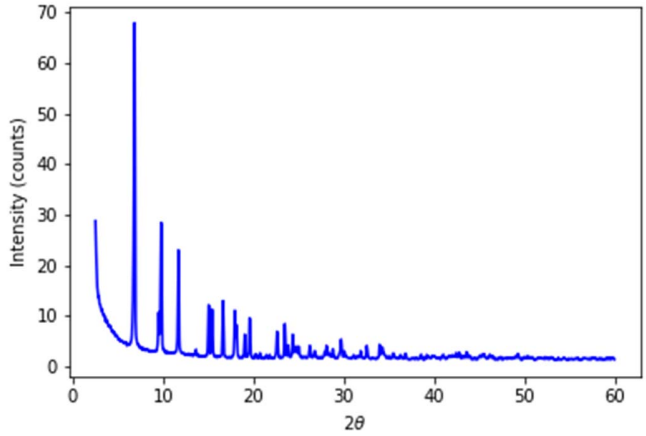
e) 7, 7, 8, 8-Tetracyanoquinodimethane



f) HKUST-1

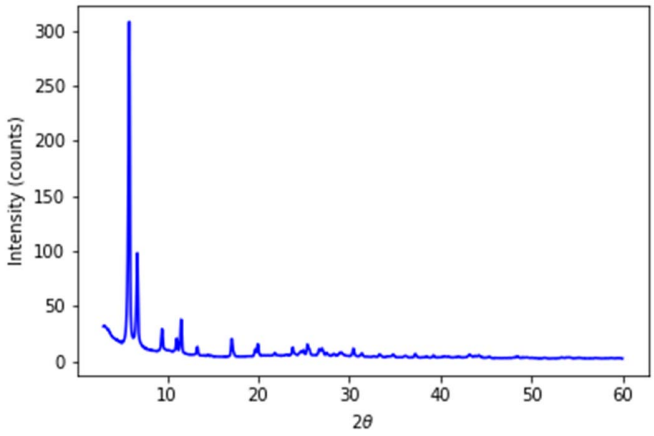


g) MIL-125-Ti-NH2



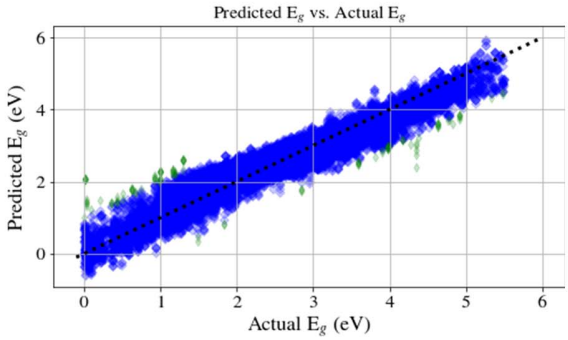
The background noise before the first peak was removed up to 2θ = 5°

h) UiO-67



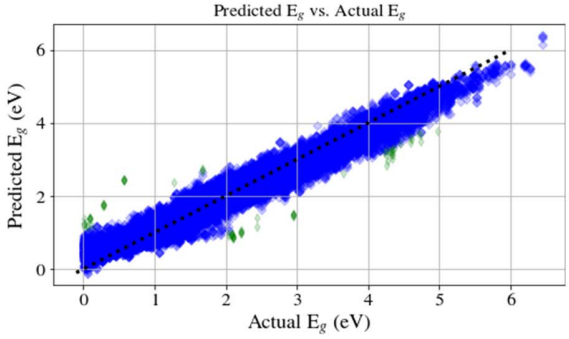
B. Plots of the assessed band-gap by the CNNs vs. the reported in the datasets with the compounds of the training set.

The plots of the left side were obtained with the CNNs that only used the diffraction patterns as input vector, whereas those in the right side were obtained with the CNNs that used both diffraction patterns and the compositional vector. The plots in the top were obtained with compounds of the QMOF. Those in the middle were plot with the compounds of the OMDB dataset. The plots in the bottom were plot with the compounds of the HSE dataset. The assessments with an absolute error AE $\leq$ 1 eV were highlighted in blue.



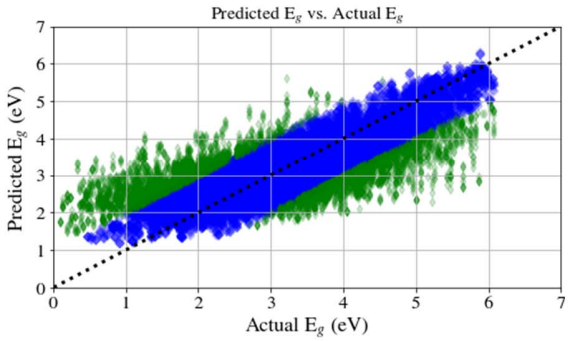
MAE = 0.213 eV

RMSE = 0.274 eV



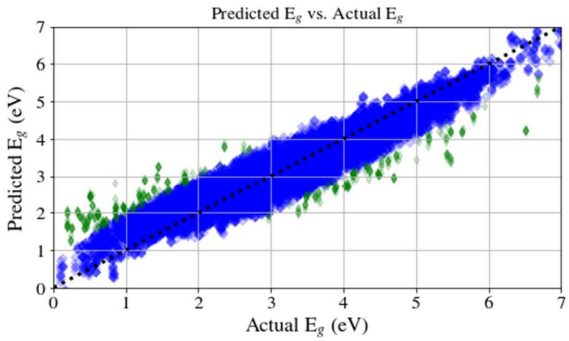
MAE = 0.190 eV

RMSE = 0.246 eV



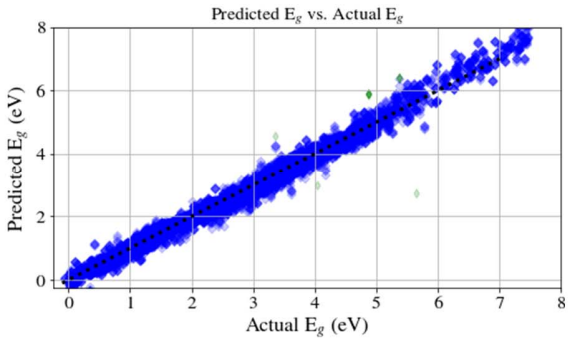
MAE = 0.483 eV

RMSE = 0.628 eV



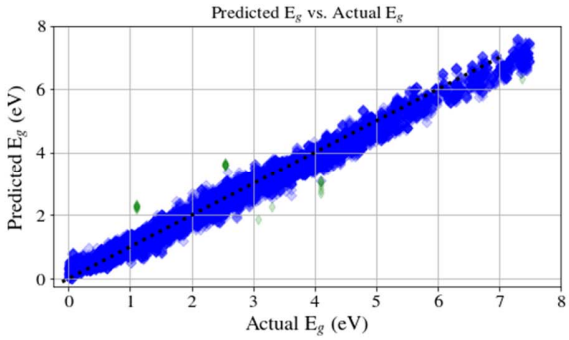
MAE = 0.255 eV

RMSE = 0.335 eV



MAE = 0.127 eV

RMSE = 0.172 eV



MAE = 0.160 eV

RMSE = 0.208 eV

C. Element abundance in the compounds of the datasets

a. QMOF

Symbol	%
H	100.00
C	100.00
O	83.15
N	82.83
Zn	17.50
Cu	17.44
S	16.86
Cd	16.12
Cl	9.98
Ag	7.16
Co	5.43
P	4.77
Mn	4.28
I	4.17
Br	4.11
F	3.68
Ni	3.51
Hg	2.51
Na	2.35
K	2.26
Pb	1.68
Fe	1.66
Li	1.62
Tb	1.60
Gd	1.48
Ca	1.48
Nd	1.25
Sm	1.24
Dy	1.15
U	1.05

La	1.04
Ba	0.97
Symbol	**%**
Mo	0.95
Er	0.92
Sn	0.91
Pr	0.90
Sr	0.89
Mg	0.81
V	0.77
B	0.70
Ho	0.64
Cs	0.57
Rb	0.46
Au	0.43
Tl	0.42
Yb	0.39
Y	0.37
Bi	0.36
Si	0.35
In	0.34
Se	0.34
Pt	0.32
Pd	0.29
Ru	0.24
Tm	0.22
Eu	0.22
Al	0.21
Ga	0.21
Cr	0.19
Rh	0.18

W	0.16
Lu	0.16
As	0.14
Sb	0.14
Symbol	**%**
Te	0.10
Ti	0.10
Sc	0.10
Zr	0.09
Th	0.06
Ce	0.05
Re	0.04
Ge	0.04
Pu	0.02
Np	0.02
Ir	0.02
Nb	0.01
Tc	0.01
Be	0.01

Next elements had an abundance lower than 0.01 %: Ra, Ac, Kr, Pa, Rn, Am, Fr, Ar, At, Po, Ne, He, Xe, Os, Ta, Hf, Pm, and Cm

b. OMDB

Symbol	%
H	100.00
C	100.00
O	75.86
N	64.13
S	11.32
Cl	9.16
Br	6.81
F	5.91
P	3.31
I	2.51
B	2.27
Si	2.14
Fe	1.51
Se	1.06
Pd	0.93
Zn	0.63
Pt	0.60
Ru	0.57
Sn	0.43
Ag	0.41
Cr	0.35
Ti	0.34
Li	0.34
Pb	0.31
W	0.31
Na	0.31
Au	0.31
Ni	0.30
Cu	0.30
Mo	0.30
Cd	0.28
Mg	0.27

Ir	0.26
Symbol	**%**
Al	0.26
Ga	0.26
Co	0.26
Ge	0.25
Hg	0.23
Rh	0.23
Te	0.22
Mn	0.22
Sb	0.18
K	0.18
Os	0.15
Re	0.15
Bi	0.14
As	0.12
Zr	0.11
In	0.10
U	0.08
Ca	0.08
Sr	0.07
Y	0.06
Tl	0.05
Cs	0.05
Ta	0.04
Ba	0.04
La	0.03
V	0.03
Rb	0.03
Nb	0.02
Be	0.02
Hf	0.02
Lu	0.02

Sc	0.01

Next elements had an abundance lower than 0.01 %: Rn, At, Tc, Fr, Ar, Ra, Ac, Kr, Th, Pa, Po, Pr, He, Nd, Xe, Ce, Yb, Tm, Er, Ho, Dy, Tb, Gd, Eu, Sm, Pm, Ne

c. HSE

Symbol	%
O	45.17
S	16.83
K	10.19
Cl	10.19
Se	9.72
Cu	9.47
P	9.23
N	8.65
Na	8.59
F	7.93
H	7.85
Ag	7.54
Ba	7.52
Cs	7.01
Te	6.43
I	6.12
As	5.94
Sb	5.61
Rb	5.53
Bi	5.14
V	4.99
Sr	4.81
Ge	4.81
Br	4.69
Mn	4.67
Li	4.58
C	4.46
Sn	4.38
Fe	4.32
Hg	4.23
Cd	4.05
Ca	4.05

Pb	4.03
Si	3.82
Tl	3.82
In	3.45
Symbol	**%**
Zn	3.37
Au	3.37
Nb	3.14
Cr	3.12
Ti	2.96
B	2.94
Ga	2.75
Mo	2.47
Al	2.45
La	2.36
Co	2.24
Pd	2.06
Mg	2.03
Ni	1.95
Ta	1.91
Pt	1.54
W	1.52
Y	1.52
Zr	1.21
Ru	0.99
Re	0.84
Lu	0.82
Hf	0.68
Os	0.60
Rh	0.53
Sc	0.47
Xe	0.45
Be	0.45

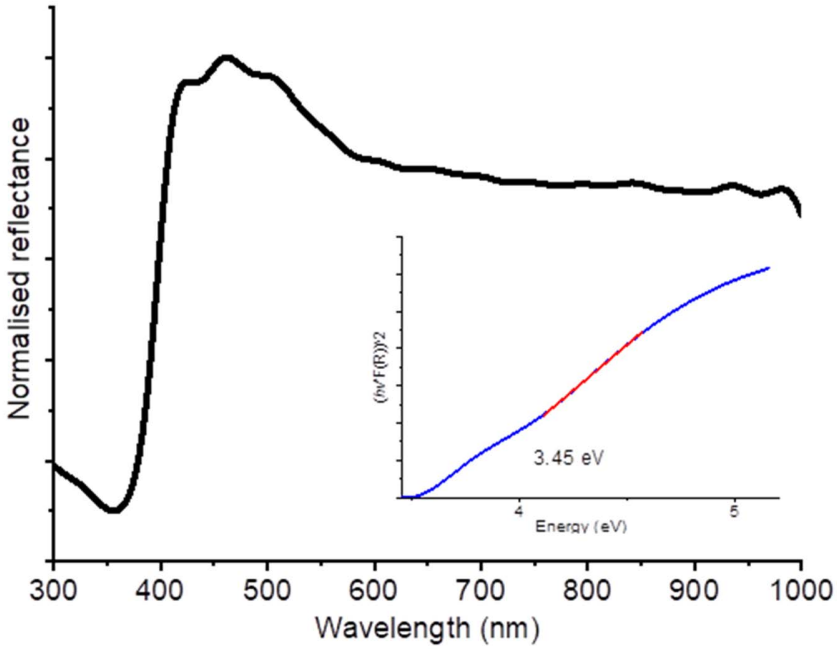
Ce	0.33
Ir	0.33
Tc	0.31
Kr	0.10

Dy	0.06
He	0.02

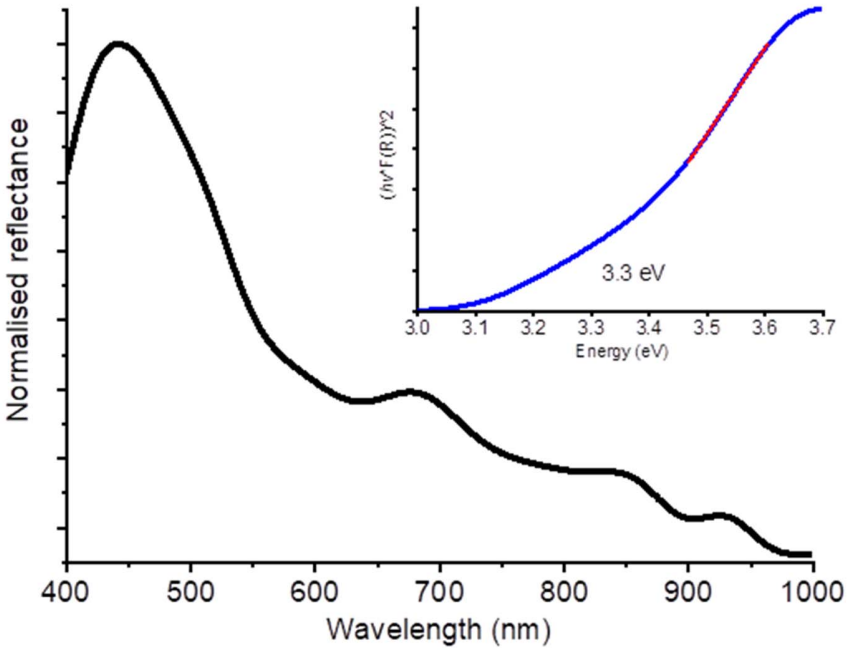
Next elements had an abundance lower than 0.01 %: Er, Pm, Ne, Ar, Pr, Nd, Sm, Tm, Eu, Gd, Tb, Ho, Yb, Po

C. Band-gap assessed by UV-visible Diffuse Reflectance Spectroscopy

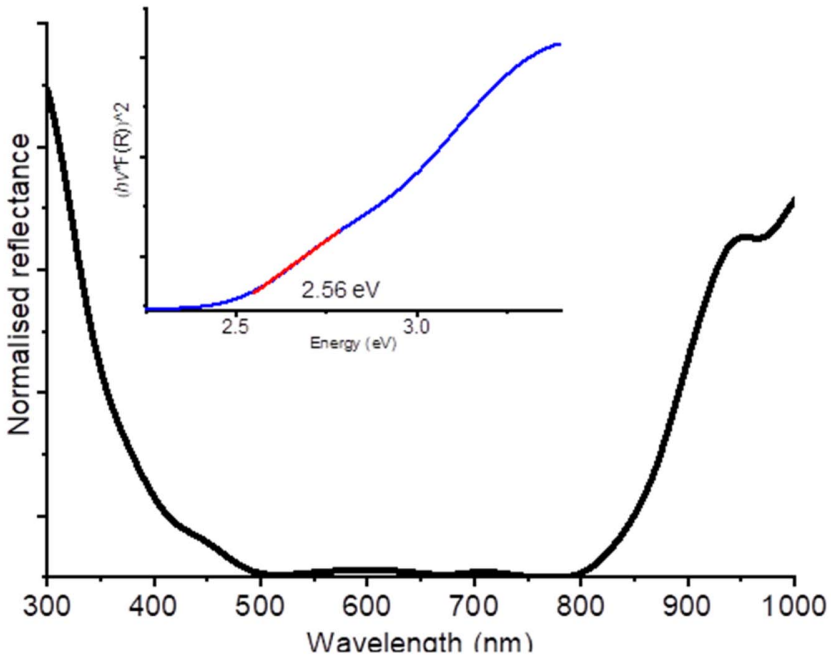
a) ZnO



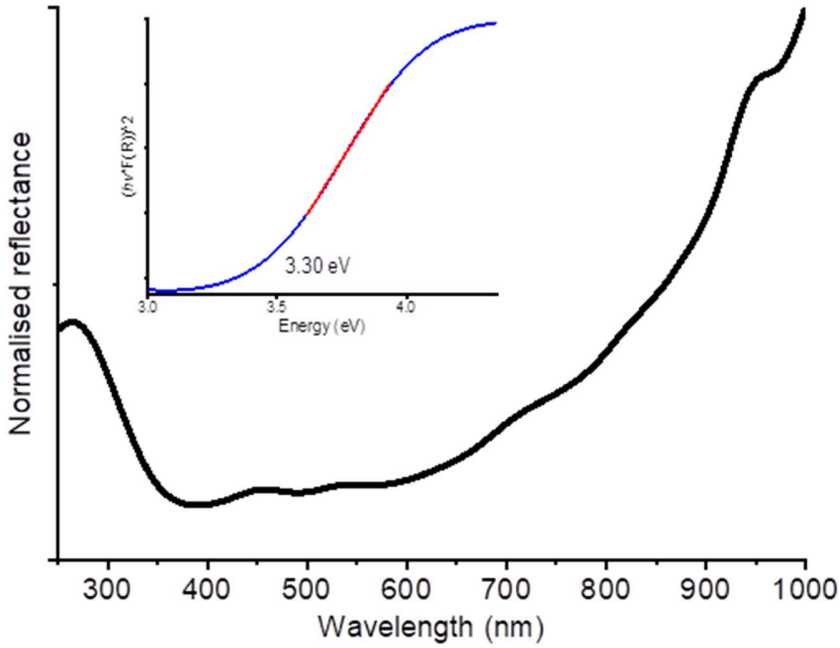
b) SnO_2



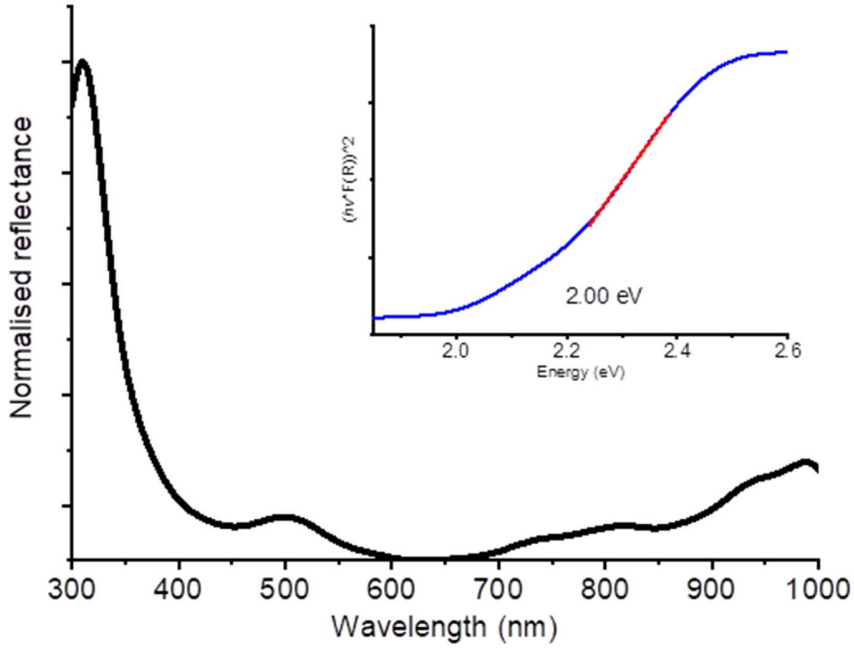
c) CuO



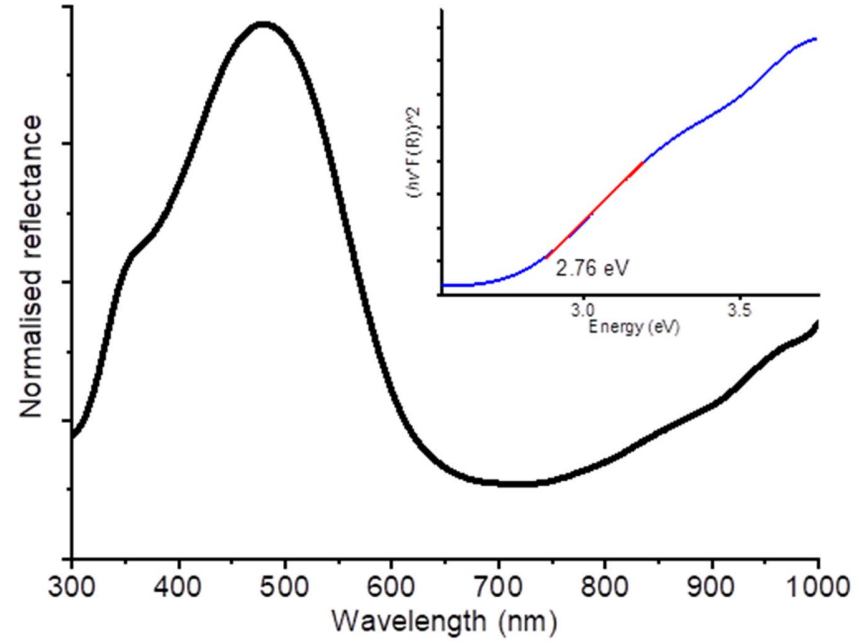
d) 1, 4, 5, 8-Naphtalenetetracarboxilic dianhydride, NTCDA



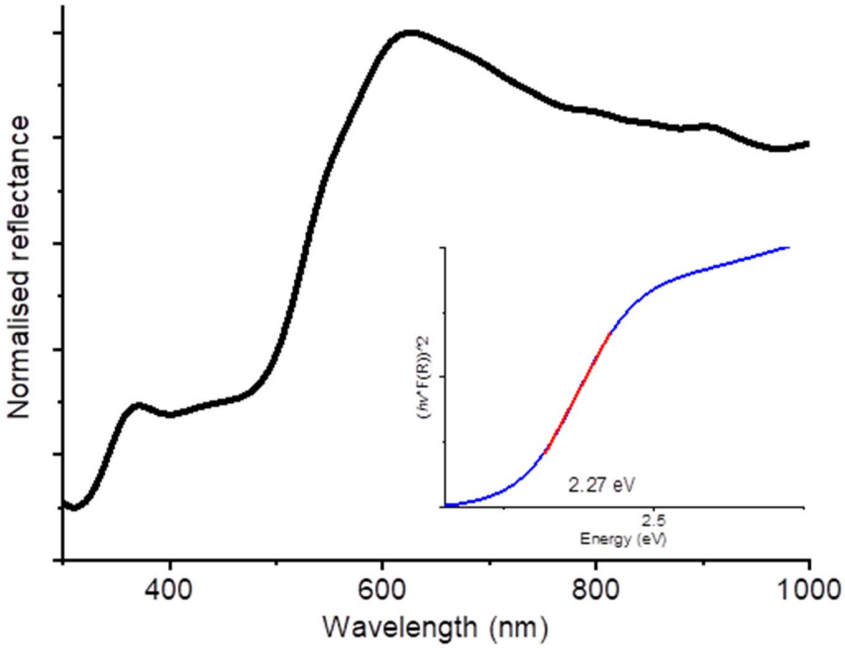
e) 7, 7, 8, 8-Tetracyanoquinodimethane



f) HKUST-1



g) MIL-125-NH_2



h) UiO-67