Supporting Information

Highly Crystalline MOF-based Materials Grown on Electrospun Nanofibers

M. Bechelany*[a], M. Drobek[a], C. Vallicari[a], A. Abou Chaaya[a], A. Julbe[a], P. Miele[a]

SI.1 Calculation of the reaction yields

x = quantity (mol) of metal in the oxide
y = quantity (mol) of metal in the MOF
A = total quantity (mol) of metal in the composite material
B = final weight (g) of the composite material
M_Wx = oxide molecular weight (g/mol)
M_Wy = MOF molecular weight (g/mol)

As far as we did not detect any metal loss from the coated nanofibers to the solution, A was considered as a constant :

$$A = x + y \qquad \text{(Eq. 1)}$$

and the final weight of the composite material can be written as :

$$B = x*M_Wx + y*M_Wy \qquad \text{(Eq. 2)}$$

By replacing (x = A – y) in (eq. 2), we obtain :

$$B = (A - y)*M_Wx + y*M_Wy = A*M_Wx - y*M_Wx + y*M_Wy = A*M_Wx + y*(M_Wy - M_Wx)$$

and thus :

$$y = (B - A*M_Wx)/(M_Wy - M_Wx)$$

The reaction yield can thus be written as follows:

$$Yield(\%) = 100*(y/A) = 100*[(B - A*M_Wx)/(M_Wy - M_Wx)]/A \qquad \text{(Eq. 3)}$$

Example of a yield calculation for a ZIF-8-based composite material :

M_W (ZnO) = 81.40 g/mol
M_W (ZIF-8) = 229.60 g/mol
When a given quantity of ZnO was deposited by ALD (e.g. m(ZnO) =2.05 mg), the corresponding value of A was calculated as follows :

$$A = 2.05\ 10^{-3}/81.40 = 2.52\ 10^{-5}\ mol$$

The weight of the final composite material after the hydrothermal conversion of ZnO to ZIF-8 was measured:

$$B = 5.55mg$$

The yield of the conversion reaction was thus calculated by Eq. 3 :

$$Y(\%) = 100*[(B - A*M_WZnO) / (M_WZIF\text{-}8 - M_WZnO)] / A$$
$$= 100*[(5.55\ 10^{-3} - 2.52\ 10^{-5} * 81.40) / (229.60 - 81.40)] / 2.52\ 10^{-5}$$
$$= 93$$