Supporting Information

Highly Crystalline MOF-based Materials Grown on Electrospun Nanofibers

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

SI.1 Calculation of the reaction yields

\[ x = \text{quantity (mol) of metal in the oxide} \]
\[ y = \text{quantity (mol) of metal in the MOF} \]
\[ A = \text{total quantity (mol) of metal in the composite material} \]
\[ B = \text{final weight (g) of the composite material} \]
\[ M_{Wx} = \text{oxide molecular weight (g/mol)} \]
\[ M_{WY} = \text{MOF molecular weight (g/mol)} \]

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

\[ A = x + y \quad \text{(Eq. 1)} \]

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

\[ B = x*M_{Wx} + y*M_{WY} \quad \text{(Eq. 2)} \]

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:

\[ y = \frac{B - A*M_{Wx}}{M_{WY} - M_{Wx}} \]

The reaction yield can thus be written as follows:

\[ \text{Yield(\%) = } 100*\frac{(y/A)}{A} = 100*\frac{(B - A*M_{Wx})/(M_{WY} - M_{Wx})}{A} \quad \text{(Eq. 3)} \]

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

\[ M_{W} (\text{ZnO}) = 81.40 \text{ g/mol} \]
\[ M_{W} (\text{ZIF-8}) = 229.60 \text{ g/mol} \]

When a given quantity of ZnO was deposited by ALD (e.g. \( m(\text{ZnO}) = 2.05 \text{ mg} \)), the corresponding value of \( A \) was calculated as follows:

\[ A = 2.05 \times 10^{-3}/81.40 = 2.52 \times 10^{-5} \text{ mol} \]

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

\[ B = 5.55 \text{ mg} \]

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

\[ Y (\%) = 100* \frac{[(B - A*M_{W}\text{ZnO})/(M_{W}\text{ZIF-8} - M_{W}\text{ZnO})]}{A} = 100* \frac{[(5.55 \times 10^{-3} - 2.52 \times 10^{-5} * 81.40)/(229.60 - 81.40)]}{2.52 \times 10^{-5}} = 93 \]