Electronic Supplementary Information for: Guest-host van der Waals interactions decisively affect the molecular transport in mesoporous media[†]

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1 Quantification of drug loading

The loading fraction is determined on the basis of weight loss during the combustion of IMC. This weight loss region is, of course, accompanied by an exothermal transition in the corresponding DSC curves. The temperature interval is determined on the basis of the derivative of the weight loss with respect to temperature and is shown in Fig. 1. The first two weight loss stages, accompanied by endothermal regions in DSC curves, are due to the removal of remaining solvents. The third and most prominent weight loss stage is due to combustion of IMC.
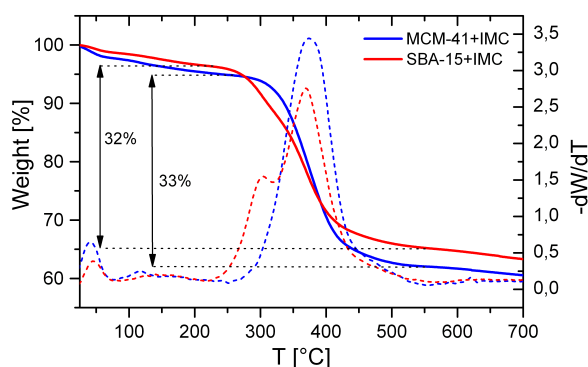
2 UV-VIS spectra of aqueous solutions of THF, IMC and THF+IMC

Since the prepared samples contain THF, we chose the wavelength 268 nm, at which THF absorption does not interfere with IMC absorption. Specifically, we prepared aqueous solutions of THF with and in absence of IMC, where the THF concentration is 410 times larger than the maximal concentration that can be achieved during drug release. The latter is determined from the first weight weight loss stages. The UV-VIS spectra are shown in Fig. 2.

Fig. 1 TGA curves and the first derivative of weight with respect to temperature for IMC loaded SBA-15 and MCM-41.
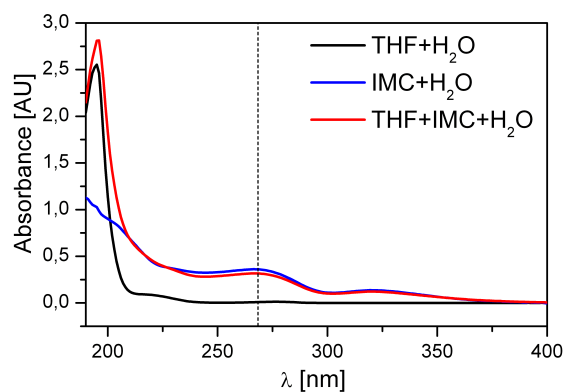

Fig. 2 UV-VIS spectra of aqueous solutions of THF, IMC and THF+IMC.

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3   Calculation of effective large-scale diffusion coefficients

As we have shown (A. Godec, T. Ukmar, M. Gaberšček, F. Merzel, *Europhys. Lett.*, 2010, **92**, 60011), the asymptotic transport on large scales can be described by means of a 1-dimensional free diffusion equation with an effective diffusion coefficient, D_{eff} which evolves from an initial box-shaped distribution ($C_{ls}(x,t=0) = C_{ls}^0$ for $|x| \leq L/2$ and 0 otherwise):

$$\frac{\partial C_{ls}}{\partial t} = D_{eff}\frac{\partial^2 C_{ls}}{\partial x^2}.$$

The solution is obtained straightforwardly by means of Laplace transformation and reads

$$C_{ls}(x,t) = \frac{1}{2}C_{ls}^0\left[\text{erf}\left(\frac{L/2-x}{2\sqrt{D_{eff}t}}\right) + \text{erf}\left(\frac{L/2+x}{2\sqrt{D_{eff}t}}\right)\right]$$

If we denote the thickness of the diffusion layer as h, the fraction of solute released is then given by $\Theta(t) = 1 - (LC_{ls}^0)^{-1}\int_{-(L/2+h)}^{(L/2+h)} C_{ls}(x,t)dx$ and can be shown to be

$$\begin{aligned}\Theta(t) = \; & 1 - \frac{(1+\frac{L}{h})\text{erf}\left[\frac{L+h}{2\sqrt{D_{eff}t}}\right] + \text{erf}\left[\frac{-h}{2\sqrt{D_{eff}t}}\right]}{4LD_{eff}t/h} \\ & - \frac{\exp\left[\frac{-(L+h)^2}{4D_{eff}t}\right] - \exp\left[\frac{-h^2}{4D_{eff}t}\right]}{2L\sqrt{\pi D_{eff}t}}.\end{aligned}$$

For $h = 0$ the above equation reduces to the result we derived in our previous work. D_{eff} is in turn obtained from $C(\mathbf{r},t)$ by fitting $\int_0^t d\tau \oint_O \mathbf{j}(\mathbf{r},\tau)\cdot d\mathbf{S}$ with the analytical expression for $\Theta(t)$ for long times. Specifically we used the last $30\cdot10^3$ steps. Note that if the large scale transport were in fact diffusive and isotropic the whole time (*i.e.* it would follow 1D diffusion with some D_{eff}), then the fraction of drug released would follow the last equation above. Only in this case, one would be allowed to replace the microscopic geometry and interactions with an effective (time independent) D_{eff}. Our results demonstrate, however, that even in absence of attractions to walls, the large scale behavior follows a 1-dimensional diffusion equation only for long t. The time domain, where the asymptotic diffusive behavior is in fact established, can be determined only *a posteriori*.